18th Biennial Intl. Conference of the APS Topical Group on Shock Compression of Condensed Matter held in conjunction with the 24th Biennial Intl. Conference of the Intl. Association for the Advancement of High Pressure Science and Technology (AIRAPT)
Seattle, Washington
http://www.aps.org/meetings/meeting.cfm?name=SHOCK13
Monday, July 8, 2013 8:00AM - 9:00AM  
Session A1 Plenary Session I  
Grand Ballroom I - Gilbert Collins, Lawrence Livermore National Laboratory

8:00AM A1.00001 Thermodynamic Paths in Planetary Collisions: Shock Vaporization of SiO₂, MgO, and Fe  
RICHARD KRAUS, Harvard University — The final stage of terrestrial planet formation is punctuated by a series of violent collisions that lead to the observed diversity of the surviving planets. These collisions are sufficiently energetic to melt and vaporize large fractions of the colliding bodies and affect their bulk composition. However, our understanding of the thermal and chemical evolution of the terrestrial planets is severely limited by our lack of knowledge of planetary materials at the conditions achieved during these giant impact events. I will describe my work to advance the state of knowledge of planet-forming minerals at the extreme states achieved during planetary collisions. I will focus on recent shock-and-release experiments performed at the Sandia Z machine under the Fundamental Science Program, where I am developing techniques to measure the temperature, density, and entropy along the liquid-vapor dome. Using magnetically accelerated flyer plates at impact velocities of tens of km/s, we can access the entire range of phase space relevant to the giant impact stage of terrestrial planet formation. Our data on SiO₂, MgO, and Fe highlight the importance of the entropy generation at high shock pressures, reveal the deficiencies of previous equation of state models, and are being used to constrain new multi-phase equations of state. I will discuss how these data will address key questions about the formation of planets inside and outside our Solar System.

8:30AM A1.00002 Jamieson Award Talk - Novel Materials Prediction and Experimental Synthesis under Pressure  
DUCKYOUNG KIM, Carnegie Institute Washington — Pressure enables us to explore entire new dimension of materials science by perturbing energy landscape of materials beyond conventional thermodynamics limits. Realization of novel functional energy materials, synthesized under pressure, to ambient conditions can provide another insight to solve current Energy Challenge. In this presentation, I will show recent progress on our theory-experiment collaborative works in this direction. Crystal structure searching using density functional theory predicts possible novel phases and guides our experiments. Experimental observations provide inputs for refinement of calculations. I will present our recent successful examples to highlight the importance of integrated experiment-theory collaboration for Energy Frontier Research.

Monday, July 8, 2013 9:15AM - 10:45AM  
Session B1 ME.4 Strength I  
Grand Ballroom I - Bruce Remington, Lawrence Livermore National Laboratory

9:15AM B1.00001 Extracting Strength from Ramp-Release Experiments on Z  
JUSTIN BROWN, Sandia National Laboratories — Releasing from a compressed state has long been recognized as a sensitive measure of a material’s constitutive response. The initial elastic unloading provides insights which can be related to changes in shear stress or, in the context of classic plasticity, to the material’s yield surface. Ramp compression and subsequent release experiments on Sandia’s Z machine typically consist of a driving aluminum electrode pushing a sample material which is backed by a window. A particle velocity measurement of the sample/window interface provides a ramp-release profile. Under most circumstances, however, the impedance mismatch at this interface results in the measurement of a highly perturbed velocity, particularly at the late times of interest. Wave attenuation, the finite pressure range over which the material elastically unloads, and rate effects additionally complicate the interpretation of the experiment. In an effort to accurately analyze experiments of this type, each of these complications is addressed. The wave interactions are accounted for through the so-called transfer function methodology and involves a coupling of the experimental measurements with numerical simulations. Simulated window velocity measurements are combined with the corresponding in situ simulations to define a mapping describing the wave interactions due to the presence of the window. Applying this mapping to the experimentally measured velocity results in an in situ sample response which may then be used in a classic Lagrangian analysis from which the strength can be extracted via the self-consistent method. Corrections for attenuation, pressure averaging, and limitations of the analysis due to rate-effects are verified through the use of synthetic data. To date, results on the strength of aluminum to 1.2MBar, beryllium to 1 MBar, and tantalum to over 2MBar have been obtained through this methodology and will be presented.

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:45AM B1.00002 Bounds on the Rate Dependent Plastic Flow of Tantalum up to 75 GPa  
BRYAN REED, REED PATTERSON, MUKUL KUMAR, Lawrence Livermore National Laboratory — We report improvements in a general thermodynamics-based velocimetry analysis method designed to extract strength and plastic-flow information from shock and ramp compression experiments. The method allows extraction of thermodynamic histories, including deviatoric stress and plastic strain, including nonsteady rate-dependent features. The improved method includes free-surface corrections for pullback waves, reduced noise sensitivity, and application to pressures of 75 GPa and higher. Specifically, we show results for shock waves in tantalum, including bounds on the plastic flow behavior at strain rates exceeding 1x10^7/s. The deviatoric stress appears to be almost entirely dependent on strain rate, with very little pressure dependence. The deviatoric stress in the post-shock plateau state appears to be very small at higher pressures, calling into question the value of considering strength as a steady-state pressure-dependent quantity.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

10:00AM B1.00003 Shear Strength Development in Tantalum Alloys: Effects of Cold Work and Alloying  
JEREMY MILLETT, GLENN WHITEMAN, NEIL BOURNE, SIMON CASE, AWE, Aldermaston, RUSTY GRAY, Los Alamos National Laboratory — The response of tantalum and its alloys during shock loading conditions is controlled largely by the motion of dislocations present within the microstructure. This has been attributed to the high Peierls stress reducing the ability of these materials to accommodate strain by the generation of additional dislocation line length. This has manifested itself in the mechanical response as a clear reduction in shear strength behind the shock front, as dislocation motion is considered a stress relief mechanism. However, it has also been shown that this shear strength reduction can itself be reduced, either by prior cold work before shock loading, or via simple alloying such as an addition of 2.5wt% tungsten. In this work, we explore these issues further by investigating the shear strength development in a cold rolled Ta2.5wt%W alloy (50% reduction in thickness) and an annealed Ta-10wt%W alloy. Results are compared to previous work on annealed tantalum and Ta-2.5wt%W, and a 50% cold rolled pure tantalum.
experiments were performed with commonly used copper powder additive and without any additives for comparison. It was shown that increase of additive

cubed phase was performed in plane recovery ampoules using high temperature shock compression method (HTSC). The samples containing different concentra-

tions of silicon nitride powder and high compressible temperature raising inert additive (KBr, KCl) were subjected to shock loading at 36 and 50 GPa. Similar

cubic phase to cubic phase occurs within 4 ns under shock compression at maximum pressure of approximately 11 GPa, showing no transient phases with available experimental

Technique — At high pressure zirconium is known to undergo a phase transformation from the hexagonal close packed (HCP) alpha phase to the simple hexagonal omega

phase. Under conditions of shock loading, the high-pressure omega phase is retained upon release. However, the hysteresis in this transformation is not well

represented by equilibrium phase diagrams and the multi-phase plasticity likely under shock conditions is not well understood. For these reasons, the influence of

peak shock stress and temperature on the retention of omega phase in Zr has been explored. In-situ VISAR and PDV measurements along with post-mortem

metallographic and neutron diffraction characterization of soft recovered specimens have been utilized to quantify the volume fraction of retained omega phase

characterize the morphology of the shocked alpha and omega phases, and qualitatively understand the kinetics of this transformation. In turn, soft recovered

samples with varying volume fractions of retained omega phase have been utilized to understand the contribution of omega and alpha phases respectively to

strength in Zr.

In-situ x-ray diffraction and electrical resistance measurements were performed simultaneously during this rapid pressure increase to provide the first time resolved data on

rapid pressure increase to provide the first time resolved data on structural phase transitions of materials under previously unexplored compression rate-pressure conditions that bridge traditional static and shock/dynamic experimental platforms.

An overall increase of copper additive concentration from 0% to 9% results in an increase in the volume fraction of retained omega phase from 22% to 40% for KBr additive and above 40% for KCl additive. In these experiments cubic phase was obtained in a nanocrystalline form. Cubic phase was not found in recovered silicon nitride after loading of samples which contained no additives.

This work was supported by RFBR, grant 12-02-00980-a.

Structural phase transition in bismuth under shock compression measured via nanosecond time-resolved X-ray diffraction — Structural phase transition in bismuth under shock compression measured via nanosecond time-resolved X-ray diffraction. KAZUTAKA NAKAMURA, JIANBO HU, Tokyo Institute of Technology, KOUEI ICHIYANAGI, The University of Tokyo, NOBUAKI KAWAI, Japan Aerospace Exploration Agency, KATSURA NORIMATSU, SHIN-ICHI HARADA, YUKI KABASAWA, DAI HORIUCHI, Tokyo Institute of Technology, SHUNSKE NOZAWA, TOKUSHI SATO, SHIN-ICHI ADACHI, High Energy Accelerator Research Organization — Structural phase transition in bismuth under laser-shock compression up to 11 GPa has been studied via nanosecond time-resolved X-ray diffraction. The nanosecond time-resolved single-shot X-ray diffraction was performed using a laser-pump and X-ray probe technique with a 100-ps X-ray pulse from the synchrotron radiation facility (Photon Factory Advanced Ring, KEK). The sample was a polycrystalline bismuth foil with the thickness of 20 micrometers. The target assembly has a plasma-confined scheme and been irradiated by a 8-ns laser pulse. The results show that the shocked bismuth undergoes a series of structural transformations involving four solid structures: the Bi-I, Bi-II, Bi-III, and Bi-V phases. The transformation form the Bi-I phase to the Bi-V phase occurs within 4 ns under shock compression at maximum pressure of approximately 11 GPa, showing no transient phases with available experimental conditions. Successive phase transformations from the high-pressure Bi-V phase to the Bi-I phase via the Bi-III and the Bi-II phases during shock release within 30 ns have also been unambiguously resolved.
10:30AM B2.00006 A multiphase equation of state for Be based on the modified mean-field potential approach. Song Haifeng, Liu Haifeng, Zhang Gongmu, Wang Cong, Sun Bo. IAPCM (Institute of Applied Physics and Computational Mathematics). IAPCM TEAM — We present a first-principles scheme to study the multiphase equation of state (EOS) for Be, based on our recently developed modified mean-field potential (MMFP) approach. We first calculate the EOS for Be of hcp and bcc structure, and then compute the melting curve of Be by using MMFP approach. At last, based on the EOS of bcc Be and melting curve and considering the effect of the melting entropy, we obtain the EOS of liquid Be. Based on the results, we obtain the multiphase EOS of Be. The calculated Hugoniot of solid and liquid phase as well as the melting curve are in agreement with available experimental data.

Monday, July 8, 2013 9:15AM - 10:45AM —
Session B3 TM First Principles Methods I Fifth Avenue - Marc Crawwell, Los Alamos National Laboratory

9:15AM B3.00001 ABSTRACT WITHDRAWN —

9:45AM B3.00002 Predicting Variable Stoichiometric Compounds under High Pressure. Qiang Zhu, Artem Oganov, SUNY-Stony Brook — Materials under pressure often exhibit exotic physical and chemical behaviors. In particular, extremely new stable compounds appear. Here, we studied the variation of stoichiometry under pressure by using the evolutionary search scheme. Two kinds of oxides (Xe-O and Mg-O) have been investigated under megabar pressures. For XeO, we predict the existence of thermodynamically stable Xe-O compounds at high pressures (XeO, XeO2 and XeO3 become stable at pressures of 83, 102 and 114 GPa, respectively). For Mg-O, our calculations find that two extraordinary compounds MgO2 and Mg3O2 become thermodynamically stable at 116 GPa and 500 GPa, respectively. Our calculations indicate large charge transfer in these oxides for both systems, suggesting that large electronegativity difference and pressure are the key factors favoring their formations. We also discuss if these oxides might exist at earth and planetary conditions.

10:00AM B3.00003 Tuning dimensionality in binary Li-B compounds and evaluating thermodynamic vs kinetic stability under pressure1. Andreas Hermann, Cornell University — The binary phase diagram of the light elements lithium and boron features an intriguing phase with a finite range of stability, LiBx with 0.8 ≤ x ≤ 1.0. The experimental hexagonal structure contains two incommensurate sub-lattices, a hexagonal lithium layer, and an array of linear boron chains. An alternative structure of almost equal energy is inspired by the AI2 structure type, and contains graphitic boron sheets interspersed by trigonal lithium layers. We present results from a computational study on this system, at atmospheric and elevated pressures. We model the tunable atomic composition and predict the disappearance of the finite stability range of LiBx at P=40GPa, where layered structures become more stable than chain-like structures across the entire composition range. Kinetic barriers are estimated and are predicted to facilitate the recovery of phases synthesized at high pressure. Up to P=70GPa, all stable structures are metallic, and trends of their electronic and dynamic properties will be discussed. At P>70GPa, structure searches reveal that stoichiometric 1:1 Li-B is most stable in the NaTl structure, with a diamondoid boron network, and becomes an insulator. The Zintl-Klemm concept helps understand the different structural choices under pressure.

1Support from EFRee, a DoE-EFRC (DESC0001057), and NSF (CHE-0910623 and DMR-0907425), is gratefully acknowledged.

10:15AM B3.00004 Monitoring bonding reconstruction across the α-cristobalite → stishovite phase transition in silica. Ángel Morales García, Departamento de Química-Física I, Universidad Complutense de Madrid, Madrid, Spain, Miguel A. Salvadó, Pilar Pertierra, J.M. Menéndez, J.M. Recio, Departamento de Química Física y Analítica, Universidad Oviedo, Oviedo, Spain, MALTA CONSOLIDER TEAM — We propose a microscopic mechanism that describes how the structure and bonding network of α-cristobalite transforms into stishovite at constant pressure and temperature. A martensitic-like approach that preserves the translational symmetry is used to modelize the simultaneous and coordinated movement of all the atoms as the transition progresses. Relevant distances and angles, cell strains, and atomic displacements across the transition path are obtained from first-principles calculations under the generalized gradient approximation of the density functional theory. A soft and symmetric energetic potential approach is used to modelize the simultaneous and coordinated movement of all the atoms as the transition progresses.

10:30AM B3.00005 Stability of Solid Oxygen at High Pressure1. Sabri Elatresh, Stanimir Bonev, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada — Despite extensive theoretical and experimental studies, the stability of solid oxygen at high pressure remains an open question. Recent experimental results proposed a new phase that is stable at finite temperature [1]; however, the evidence is not conclusive. In this work, we reexamine the stability of the phase diagram of solid oxygen up to 100 GPa. In particular, we focus on the mechanical and thermodynamic stability of the recently proposed finite temperature phase. The influence of exchange interactions and the role of ion dynamics, including quantum effects, will be discussed.


1Work supported by NSERC and Acenet.

Monday, July 8, 2013 9:15AM - 10:45AM —
Session B4 MB Biology Under Extreme Conditions Vashon - Chiara Bo, Imperial College London
9:15AM B4.00001 Survival of Shewanella Oneidensis MR-1 to GPa pressures¹, RACHEL HAZEL, FABRIZIA FOGLIA, University College London, JAMES LEIGHT, GARETH APPLEBY-THOMAS, Cranfield University, ISABELLE DANIEL, Laboratoire de Géologie de Lyon, DANI EAKINS, Imperial College London, FILIP MEERSMAN, PAUL MCMILLAN, University College London — Most life on Earth is thought to occupy near-surface environments under relatively mild conditions of temperature, pressure, pH, salinity etc. That view is changing following discovery of extremophile organisms that prefer environments based on high or low T, extreme chemistries, or very high pressures. Over the past three decades, geomicrobiologists have discovered an extensive subsurface biosphere, that may account for between 1/10 to 1/3 of Earth’s living biomass. We subjected samples of Shewanella oneidensis to several pressure cycles to examine its survival to static high pressures to above 1.5 GPa. Shewanella forms part of a genus that contains several piezophile species like S. violacea and S. benthica. We have obtained growth curves for populations recovered from high P conditions and cultured in the laboratory, before being subjected to even higher pressures. We have also carried out dynamic shock experiments using a specially designed cell to maintain high-P, low-T conditions during shock-recovery experiments and observe colony formation among the survivors. Colony counts, shape and growth curves allow us to compare the static vs dynamic pressure resistance of wild type vs pressure-adapted strains.

¹Leverhulme

9:30AM B4.00002 Tolerance of budding yeast Saccharomyces cerevisiae to ultra high pressure, FUMIHISA ONO, Department of Applied Science, Okayama University of Science, MICHIKO SHIBATA, MOTOKI TORIGOE, YUTA MATSUMOTO, SHINSUKE YAMAMOTO, Okayama Ichinomiya Senior High School, NOBORU TAKIZAWA, Department of Applied Chemistry and Biotechnology, Okayama University of Science, YOSHIO HADA, Department of Biosphere-Geosphere System Science, Okayama University of Science, YOSHIHISA MORI, KENICHI TAKARABE, Department of Applied Science, Okayama University of Science — In our previous studies on the tolerance of small plants and animals to the high hydrostatic pressure of 7.5 GPa, it was shown that all the living samples could be borne at this high pressure, which is more than one order of magnitude higher than the proteic denaturation pressure. To make this inconsistancy clear, we have extended these studies to a smaller sized fungus, budding yeast Saccharomyces cerevisiae. A several pieces of budding yeast (dry yeast) were sealed in a small teflon capsule with a liquid pressure medium fluorinate (PC72, Sumitomo 3M), and exposed to 7.5 GPa by using a cubic anvil press. The pressure was kept constant for various duration of time from 2 to 24 h. After the pressure was released, the specimens were brought out from the teflon capsule, and they were cultivated on a potato dextrose agar (PDA). It was found that the budding yeast exposed to 7.5 GPa for up to 6 h showed multiplication. However, those exposed to 7.5 GPa for 12 and 24 h were found dead. The high pressure tolerance of budding yeast is weaker than that of tardigrades.

9:45AM B4.00003 The Limits of Life in the Deep Subsurface - Implications for the Origin of Life, JOHN BAROSS, University of Washington — There are very few environments on Earth where life is absent. Microbial life has proliferated into habitats that span nearly every imaginable physico-chemical variable. Only the availability of liquid water and temperature are known to prevent the growth of organisms. The other extreme physical and chemical variables, such as pH, pressure, high concentrations of solutes, damaging radiation, and toxic metals, are life-prohibiting factors for most organisms but not for all. The deep subsurface environments span all of the extreme conditions encountered by life including habitat conditions not yet explored, such as those that combine high temperature, high and low pH and extreme pressures. Some of the “extremophile” microorganisms inhabiting the deep subsurface environments have been shown to be among the most “ancient” of extant life. Their genomes and physiologies have led to a broader understanding of the geological settings of early life, the most ancient energy pathways, and the importance of water/rock interactions and tectonics in the origin and early evolution of life. The case can now be made that deep subsurface environments contributed to life’s origin and provided the habitat(s) for the earliest microbial communities. However. It can now be made that deep subsurface environments contributed to life’s origin and provided the habitat(s) for the earliest microbial communities. However, for further understanding on the role of moderate to high pressures and temperatures on the chemical and biochmical “steps” leading to life, and on the evolution and physiology of both ancient and present-day subsurface microbial communities.

10:15AM B4.00004 Analysis of barosensitive mechanisms in yeast for Pressure Regulated Fermentation, KAZUKI NOMURA, HITOSHI IWASHASHI, Gifu University, AKINORI IGUCHI, TORU SHIGEMATSU, Niigata University of Pharmacy and Applied Life Sciences — Introduction: We are intending to develop a novel food processing technology, Pressure Regulated Fermentation (PReF), using pressure sensitive (barosensitive) fermentation microorganisms. Objectives of our study are to clarify barosensitive mechanisms for application to PReF technology. We isolated Saccharomyces cerevisiae barosensitive mutant a924E1 that was derived from the parent KA31a. Methods: Gene expression levels were analyzed by DNA microarray. The altered genes of expression levels were classified according to the gene function. Mutated genes were estimated by mating and producing diploid strains and confirmed by PCR of mitochondrial DNA (mtDNA). Results and Discussion: Gene expression profiles showed that genes of ‘Energy’ function and that of encoding protein localized in “Mitochondria” were significantly down regulated in the mutant. These results suggest the respiratory deficiency and relationship between barosensitivity and respiratory deficiency. Since the respiratory functions of diploids showed non Mendelian inheritance, the respiratory deficiency was indicated to be due to mtDNA mutation. PCR analysis showed that the region of COXI locus was deleted. COXI gene encodes the subunit 1 of cytosome c oxidase. For this reason, barosensitivity is strongly correlated with mitochondrial functions.

10:30AM B4.00005 Quasi-Elastic Neutron Scattering: an insight into life at extreme conditions¹, FABRIZIA FOGLIA, RACHEL HAZEL, University College London, IOVANNA SIMEOINI, TUM - FRM II, MARIE-SOUSAI APPAVOU, Forschungszentrum Jülich GmbH, FILIP MEERSMAN, University College London, ISABELLE DANIEL, Laboratoire de Géologie de Lyon, TREVOR FORSYTH, Life Sciences Group, ILL and EPSAM/ISTM, PAUL MCMILLAN, University College London — Microbes have been found to thrive in diverse environments characterised by a wide range of pressure-temperature-composition conditions. The range of physicochemical conditions under which microbial life has been observed has continually expanded as microbiologists explore additional remote and apparently hostile environments. The studies provide us with clues about the current extent of biological organisms and allow us to explore the fundamental limits to survival of bacterial life forms under extreme conditions. We are developing quasi-elastic neutron scattering (QENS) studies to help us to understand the dynamic processes associated with H-/D-containing microbes under high P conditions. We have begun our study using samples of Shewanella oneidensis. We obtained pioneering QENS experiments at the high resolution TOFTOF spectrometer station. Our initial results show clear P dependence of H2O/D2O transfer dynamics across the bacterial cell walls.

¹DCO


9:15AM B5.00001 Carbon allotropes, MIGUEL A.L. MARQUES, University of Lyon —
dominant at higher pressure. After correction from their Raman cross-sections, the relative amounts of dissolved carbonate and bicarbonate were estimated from

were recorded using a LabRam HR800 Raman spectrometer (Horiba Jobin-Yvon) coupled to a Spectra Physics Ar laser. At equilibrium with an aragonite crystal, the Raman data show that bicarbonate is the most abundant species in low-pressure fluids below 4 GPa whereas carbonate becomes progressively dominant at higher pressure. After correction from their Raman cross-sections, the relative amounts of dissolved carbonate and bicarbonate were estimated from the areas of the ν1 and ν5 symmetric stretching Raman modes of the carbonate and bicarbonate ions, respectively. The presence of sodium chloride extends the pressure range of predominance for bicarbonate species in the fluid. The Raman data were also used to constrain a theoretical thermodynamic model of the fluid speciation in equilibrium with CaCO3. Revised thermodynamic properties of aqueous CO2 and HCO3− data for the aqueous CaHCO3− complex from 4 to 90◦ C, and estimated dielectric constants of water, enabled an equation of state characterization of the standard Gibbs free energy of CaHCO3− at the conditions of the Raman study. At 300-500◦ C, the Raman speciation results were used to constrain equilibrium constants involving the carbonate ion. The results indicate that CO2 is a minor species in fluids in equilibrium with aragonite at 300-500◦ C and P > 1 GPa. Instead, the CaHCO3− species becomes important at high pressures until carbonate ion becomes the dominant C-species.

1The authors gratefully acknowledge the support of the Deep Carbon Observatory
2co-authors: Sebastien Faq (Universite Lyon1 - Laboratoire de Geologie de Lyon); Dimitri Sverjensky (The John Hopkins University, Carnegie Institution of Washington)

Monday, July 8, 2013 9:15AM - 10:45AM — Session B6 ME.1 Particulate/Porous Materials I Cascade II - Brandon Lalone, United States Department of Energy

9:15AM B6.00001 The Sakharov Experiment Revisited for Granular Materials1, TRACY VOGLER, Sandia National Laboratories — Sakharov and co-workers in 1965 proposed an experiment in which a sinusoidal perturbation in a planar wave evolves as it travels through a material. More recent, Liu and co-workers utilized gas gun techniques rather than explosives to drive the shock wave, resulting in a better defined input. The technique has been applied to liquids such as water and mercury as well as solids such as aluminum. All analyses of the experiments conducted to date have utilized a viscous fluid approach, even for the solids. Here, the concept of the decay of a perturbation in a shock wave is revisited and applied to granular materials. Simulations utilizing continuum models for the granular materials as well as mesoscale models in which individual particles are resolved are utilized. It is found that the perturbation decay is influenced by the strength (deviatoric behavior) used in the continuum model. In the mesoscale calculations, the simulation parameters as well as the computational approach influence the results. Finally, initial experimental results for the technique using granular tungsten carbide are presented.

1Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:30AM B6.00002 Shock Propagation and Attenuation in Green River Oil Shale, DENNIS GRADY, Applied Research Associates — Shock waves produced by planar impact of thin plates onto samples of oil shale are monitored with time-resolved velocity interferometer diagnostics. Peak shock stresses are below the Hugoniot elastic limit. Stress wave measurements at successive sample thickness are analyzed to determine the experimental shock energy attenuation with propagation distance. Shock attenuation is attributed to stress wave scattering at planes of oil shale kerogen within the shale matrix. Wave scattering from planar defects is evaluated from a shock physics perspective and a scattering model is constructed that sensibly reproduces the experimental measurements of shock energy attenuation in oil shale.

9:45AM B6.00003 Theoretical Equations of State for Porous/Granular Materials1, JONATHAN BOETTGER, Los Alamos National Laboratory — Although the equation of state (EOS) for a porous/granular material is identical to the EOS for the equivalent non-porous material, the requirement that the EOS must provide a realistic model of the material in its porous/granular state adds additional challenges for EOS modelers. These difficulties can be divided into two broad categories. First, dynamic processes often drive porous/granular materials through regions of thermodynamic phase space that are poorly described by standard wide-ranging tabular EOS. Second, for materials that are only available in a granular form, it can be difficult to accurately measure the material properties/parameters that are routinely used to constrain a theoretical EOS. This talk will attempt to describe in some detail the many challenges posed to EOS modelers by porous/granular materials.

1Work supported by the U.S. Dept. of Energy under contract DE-AC52-06NA25396.

10:15AM B6.00004 Dynamic High-Pressure Behavior of Customized Silica Sand and Natural Moist Sandy Soil, GREGORY KENNEDY, NARESH THADHANI, Georgia Institute of Technology, Material Science and Engineering — The dynamic high-pressure behavior of two sets of sand based materials is presented. Sand and sandy soils with a wide range of properties have been studied in previous literature. Sand is a broad term that is applied to a wide range of geologic materials found in nature. This work investigates one complicated system, a natural sandy soil with an 8% water content pressed to 1.7g/cm3, and a customized high purity silica sand with rounded grains and controlled size, size distribution and water content. The customized sand was selected with two size ranges, approximately 50µm and 500µm, to provide a range of responses to compare with meso-scale simulations. The materials were pressed into a copper capsule ring connected to a copper driver plate and backed by a PMMA window. Experiments were performed in plate impact high velocity gas gun, using VISAR velocity interferometry and PVDF piezoelectric pressure gauges. The shock velocity was calculated from transit times measured from velocity profiles recorded by VISAR probes at the back surface of the driver and the rear surface of the sample in contact with the PMMA window. PVDF pressure gauges were used in some experiments to compare with the VISAR records.
10:30AM B6.00005 The effect of phase transition on the failure behaviors of PZT 95/5 under shock compression, FUPING ZHANG, HONGLIANG HE, GAOMIN LIU, YUSHENG LIU, Institute of Fluid Physics, P. O. Box 919-102, Mianyang, Sichuan 621900, People’s Republic of China — PZT 95/5 ferroelectric ceramics has been utilized for the use in shock driven pulsed power supplies for many years. In previous studies, the low impendence failure layer had been confirmed in PZT 95/5 when the shock pressure is up to 2.4 GPa. But to the shock compression of the poled PZT 95/5, the failure behavior of this material is still unknown. In this paper, the failure behaviors of axially poled PZT 95/5 have been tested by measuring the particle velocity of the rear free surface at different pressures. Results show that the failure layer exists in poled PZT 95/5 when the shock pressure reaches 2.4 GPa. Through analysis the velocity profile of free surface, which shows that the velocity of failure layer is the same as the shock-wave speed and the delay time decreases with increasing the shock stress. Comparing the failure behaviors of unpoled PZT 95/5, it finds that the threshold pressure and the velocity failure layer are the same, but the delay time in poled PZT 95/5 is slightly higher than that in unpoled PZT 95/5. The FE to AFE phase transition has been suggested to explain the increase of the delay time in poled PZT 95/5.

Monday, July 8, 2013 11:00AM - 12:30PM –
Session C1 ME 4 Strength II Grand Ballroom I - Eric Brown, Los Alamos National Laboratory

11:00AM C1.00001 Structure shocks at ultrahigh strain rates: what can they tell us about material behavior on very fast time scales?, JONATHAN CROWHURST, Lawrence Livermore National Laboratory — In recent years, techniques based on table-top laser systems have shown promise for investigating dynamic material behavior at high rates of both compressive and tensile strain. Common to these techniques is a laser pulse that is used in some manner to rapidly deliver energy to the sample; while the energy itself is often comparatively very small, the intensity can be made high by tightly focusing the pump light. In this way pressures or stresses can be obtained that are sufficiently large to have relevance to a wide range of basic and applied fields. Also, when combined with established ultrafast diagnostics these experiments provide very high time resolution which is particularly desirable when studying, for example shock waves, in which the time for the material to pass from undisturbed to fully compressed (the “rise time”) can be extremely short (order 10 ps or less) even at fairly small peak stresses. Since much of the most interesting physics comes into play during the rise time, it is important to be able to resolve the rise time. In this context I will discuss shock measurements on aluminum and iron thin films and compare the results with known behavior observed at lower strain rates. Specifically, for aluminum, I will compare our assessed steady wave data at strain rates of up to \(10^{10}\) s\(^{-1}\) to literature data up to \(\sim10^{-9}\) s\(^{-1}\) and show that the well-known fourth power scaling relation of strain rate to shock stress is maintained even at these very high strain rates. For iron, I will show how we have used our nonsteady data (up to \(\sim10^9\) s\(^{-1}\)) to infer a number of important properties of the alpha to epsilon polymorphic transition. 1. The transition can occur on the tens of ps time scale at sufficiently high strain rates and correspondingly very large deviatoric stresses, and 2. most of the material appears to transform at a substantially higher stress than the nominal value usually inferred from shock wave experiments of about 13 GPa. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 with Laboratory directed Research and Development funding (12ERD042), as well as being based on work supported as part of the EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award No. DESC001057.

11:30AM C1.00002 On the weak shock limit (WSL) in condensed matter, NEIL BOURNE, AWE Aldermaston Reading Berkshire RG7 4PR — The response of materials under shock encompass a range of pressure levels that span a region from the elastic limit up to the finis extremis at which the material enters the warm dense matter regime. Between these bounds the material spans two distinct regimes characterized by different wave profiles and responses. These are general known as the strong shock and weak shock regimes. The boundary between these is simply described by the overtake of the shock over the elastic wave to form a single rather than a two-wave structure. However this threshold corresponds to a change from an unsteady region to a single zone that corresponds to a series of physical thresholds being exceeded. This paper describes some of these and explores their consequences upon observed response with emphasis on steady and unsteady regions at relevant length scales.

11:45AM C1.00003 Dynamic Strength of Tantalum under impact, BENNY GLAM, MEIR WERDIGER, Applied Physics Division, Soreq NRC, 81800 Yavne, Israel, SHLOMI LEVI PISTINNER, Nuclear Physics and Engineering Division, Soreq NRC, 81800 Yavne, Israel — Plane impact experiments of double shock and shock-fragmentation in Tantalum were carried out in a gas gun. VISAR diagnostics has been implemented to measure the particle velocity and the free surface velocity. The VISAR information was utilized to study the dynamic strength of Tantalum under compression and tension. The pressure in the experiments was below 35 GPa. In this pressure range the dominant mechanism is expected to be dislocation motion. A 1-d hydrodynamic code was used in order to match various strength models. As expected, both the Johnson-Cook and the Guinan-Steinberg models do not reproduce the experimental results. Therefore in this paper we compare the Zerilli-Armstrong model which has been recently calibrated at strain rate of 6x10^9 s\(^{-1}\) using the split Kowalsky-Hopkinson bar to our experimental results at strain rate of 10^9 s\(^{-1}\).

12:00PM C1.00004 Laser Compression of Nanocrystalline Tantalum, CHIA-HUI LU, University of California, San Diego, BRUCE REMINGTON, BRIAN MADDOX, LLNL, BIMAL KAD, University of California, San Diego, HYE-SOOK PARK, LLNL, MEGUMI KAWASAKI, Hanyang University, TERENCE LANGDON, University of Southern California, MARC MEYERS, University of California, San Diego — Nanocrystalline tantalum (g.s. ∼ 70 nm) prepared by severe plastic deformation (HPT) from monocrystalline [100] stock was subjected to high energy laser driven shock compression (up to ∼850 GPa), generating a pressure pulse with initial duration of 3 ns and amplitude of up to ∼145 GPa. TEM revealed few dislocations within the grains and an absence of twins in the shock strengths, in contrast with monocrystalline tantalum, which exhibited twinning at P > ∼45 GPa. Hardness measurements were conducted and show a rise as the energy deposition surface is approached, evidence of shock-induced defects. The grain size was found to increase at a distance of 100 μm from the energy deposition surface as a result of thermally induced grain growth. Calculations using the Hu-Rath analysis are consistent with the experimental results. The experimentally measured dislocation densities and threshold stress for twinning are compared with predictions using analyses based on physically-based constitutive models. The predicted threshold stress for twinning increases from ∼45 GPa for the monocrystalline to ∼165 GPa for the nanocrystalline tantalum.

12:15PM C1.00005 On the residual yield stress of shocked metals, DAVID CHAPMAN, DANIEL EAKINS, Institute of Shock Physics, Imperial College London, London, SW7 2AZ, United Kingdom, ANDREY SAVINYKH, GENNADY GARKUSHIN, Institute of Problems of Chemical Physics of Russian Academy of Sciences, Chernogolovka, 142432 Russia, GENNADY KANEL, Joint Institute for High Temperatures of Russian Academy of Sciences, Chernogolovka, 142432 Russia — The measurement of the free-surface velocity is commonly employed in planar shock-compression experiments. It is known that the peak free-surface velocity of a shocked elastic-plastic material should be slightly less than twice the particle velocity behind shock front: this difference being proportional to the yield stress. Precise measurement of the free-surface velocity can be a rich source of information on the effects of time and strain on material hardening or softening. With this objective, we performed comparative measurements of the free-surface velocity of shock loaded aluminium AD1 and magnesium alloy Ma2 samples of various thicknesses in the range 0.2mm to 5mm. We observed the expected hysteresis in the elastic-plastic compression-unloading cycle for both AD1 and Ma2, where qualitatively the peak free-surface velocity increased with increasing specimen thickness. However, the relative change in magnitude of hysteresis as function of specimen thickness observed for the Ma2 alloy was smaller than expected given the large observed change in the precursor magnitude. We propose that softening due to multiplication of dislocations is relatively large in Ma2 and results in a smaller hysteresis in the elastic-plastic cycle.
Finally, I briefly consider the challenge of comparing a full-density EOS to highly porous Hugoniot data. 1

...regime for use as an impedance match standard...solid phase and the liquid. After quickly summarizing the standard models we use in each phase, I discuss challenges unique to the multiphase construction. National Laboratory...I describe the construction of a theoretical equation of state (EOS) for cerium (IV) oxide, CeO$_2$ as well as expansion under uniaxial strain condition than that for the uniaxial stress condition. Examination of elastic stability conditions suggests that for \[001\] compressive loading, the compressive strength and tensile strength of MgO single crystal subjected to uniaxial compressive and tensile loading along \[001\] direction under two deformation conditions, namely uniaxial strain condition and uniaxial stress condition. Examination of elastic stability conditions suggests that for \[001\] compressive loading, the MgO fails mechanically due to shear instability, whereas for expansion it fails due to vanishing of tensile modulus. The ideal compressive strength under uniaxial strain condition and uniaxial stress condition is determined to be 293 GPa and 123 GPa, respectively. However, ideal tensile strength is evaluated to be \(-201 \) GPa and \(-111 \) GPa, respectively, for two loading conditions. Our results suggest that MgO single crystal offers higher resistance against failure for compression as well as expansion under uniaxial strain condition than that for the uniaxial stress condition.

...1Sandia is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the US Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

...11:30AM C2.00003 The phase diagram and transport properties of MgO from theory and experiment...LUKE SHULENBURGER, Sandia National Laboratories — Planetary structure and the formation of terrestrial planets have received tremendous interest due to the discovery of so called super-earth exoplanets. MgO is a major constituent of Earth’s mantle, the rocky cores of gas giants and is a likely component of the interiors of many of these exoplanets. The high pressure - high temperature behavior of MgO directly affects equation of state models for planetary structure and formation. In this work, we examine MgO under extreme conditions using experimental and theoretical methods to determine its phase diagram and transport properties. Using plate impact experiments on Sandia’s Z facility the solid-solid phase transition from B1 to B2 is clearly determined. The melting transition, on the other hand, is subtle, involving little to no signal in us-up space. Theoretical work utilizing density functional theory (DFT) provides a complementary picture of the phase diagram. The solid-solid phase transition is identified through a series of quasi-harmonic phonon calculations and thermodynamic integration, while the melt boundary is found using phase coexistence calculations. One issue of particular import is the calculation of reflectivity along the Hugoniot and the influence of the ionic structure on the transport properties. Particular care is necessary because of the underestimation of the band gap and attendant overestimation of transport properties due to the use of semi-local density functional theory. We will explore the impact of this theoretical challenge and its potential solutions in this talk. The integrated use of DFT simulations and high-accuracy shock experiments together provide a comprehensive understanding of MgO under extreme conditions.

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...12:00PM C2.00004 Ab-initio calculations of high pressure equation of state and ideal strength of MgO...D. MUKHERJEE, K.D. JOSHI, S.C. GUPTA, Bhabha Atomic Research Centre, Mumbai, India - 400085 — Isotherm at 0 K of fcc MgO is determined from ab-initio calculations and used to derive the 300 K isotherm, isentrope and Hugoniot of MgO. The shock parameters C and s obtained from theoretical Hugoniot are 6.74 km/s and 1.23 as compared to the experimental values of 6.87 km/s and 1.24, respectively. Further, we have determined ideal compressive strength and tensile strength of MgO single crystal subjected to uniaxial compressive and tensile loading along [001] direction under two deformation conditions, namely uniaxial strain condition and uniaxial stress condition. Examination of elastic stability conditions suggests that for [001] compressive loading, the MgO fails mechanically due to shear instability, whereas for expansion it fails due to vanishing of tensile modulus. The ideal compressive strength under uniaxial strain condition and uniaxial stress condition is determined to be 293 GPa and 123 GPa, respectively. However, ideal tensile strength is evaluated to be \(-201 \) GPa and \(-111 \) GPa, respectively, for two loading conditions. Our results suggest that MgO single crystal offers higher resistance against failure for compression as well as expansion under uniaxial strain condition than that for the uniaxial stress condition.

...12:15PM C2.00005 A multiphase equation of state for cerium (IV) oxide...ERIC CHISOLM, Los Alamos National Laboratory — I describe the construction of a theoretical equation of state (EOS) for cerium (IV) oxide, CeO$_2$, that includes a low- and high-pressure solid phase and the liquid. After quickly summarizing the standard models we use in each phase, I discuss challenges unique to the multiphase construction. I also describe some physical issues that appear in the Ce$_2$O$_7$ group of materials, including the possibility that CeO$_2$ changes chemical identity before melt. Finally, I briefly consider the challenge of comparing a full-density EOS to highly porous Hugoniot data.
to the previously predicted BC8 phase. In this transition, 3 cell-angles concurrently increase from 90 different trekking routes. We have applied FEST to carbon at 1.2 TPa and at 300 K, and successfully obtained the transition from the cubic diamond phase by flipping the inverted force at the ridge of GFES. The details of GFES around the starting local minimum are more correctly obtained by more investigating local minimum by following the inversion of the driving force acting on the simulation cell. Then, the system descends it toward a neighboring local minimum of Carbon above 1 TPa.

11:30AM C3.00002 Crystal Structure Searching by Free Energy Surface Trekking: Application to Carbon above 1 TPa, TAKAHIRO ISHIKAWA, Center for Quantum Science and Technology under Extreme Conditions, Osaka University, NAOSHI SUZUKI, Department of Pure and Applied Physics, Faculty of Engineering Science, Kansai University, KATSUYA SHIMIZU, Center for Quantum Science and Technology under Extreme Conditions, Osaka University — Crystal structure determination of materials under extreme conditions has been one of grand challenges in high-pressure materials science. In computer simulations, the crystal structure searching is carried out by exploring Gibbs free energy surface (GFES) at given pressures and temperatures. Here, we propose a new crystal structure searching technique named as free energy surface trekking (FEST). FEST is based on a very simple idea and consists of an ascent-run and a descent-run. In the ascent-run, the system is forced to ascend GFES from a starting local minimum by following the inversion of the driving force acting on the simulation cell. Then, the system descends it toward a neighboring local minimum by flipping the inverted force at the ridge of GFES. The details of GFES around the starting local minimum are more correctly obtained by more investigating different trekking routes. We have applied FEST to carbon at 1.2 TPa and at 300 K, and successfully obtained the transition from the cubic diamond phase to the previously predicted BC8 phase. In this transition, 3 cell-angles concurrently increase from 90° to 101° in the ascent-run and become 109° through the descent-run, in which the activation energy is approximately 0.17 Ry/atom.

11:45AM C3.00003 Theoretical and Experimental Study of A$_2$B$_5$O$_{12}$ Garnets Under High Pressure, ALFONSO MUNOZ, Departamento de Física Fundamental II, IMN, Universidad de La Laguna, Spain, VIRGINIA MONTESEGURO, Departamento de Física Fundamental, Electrónica y Sistemas, Universidad de La Laguna, Spain, PLACIDA RODRIGUEZ-HERNANDEZ, Departamento de Física Fundamental II, IMN, Universidad de La Laguna, Spain, FRANCISCO JAVIER MÁNJON, IDPFA Univ. Politécnica de Valencia. 46022 Valencia, Spain, VICTOR LAVIN, Departamento de Física Fundamental, Electrónica y Sistemas, Universidad de La Laguna, Spain, MALTA CONSOLIDER TEAM TEAM, MAT2010-21270-C04-02/03/04 COLLABORATION, CSD2007-0045 COLLABORATION — In the last years oxide garnets are being used for technological applications in the field of solid state materials, especially as active matrices for lasers. Features such as high thermal conductivity, hardness, and chemical and mechanical stability make them good host matrices for luminescent Rare Earth (RE$^{3+}$) ions. In this sense, large efforts have been spent to investigate the luminescence properties of (RE$^{3+}$) doped nano-structured garnets, especially in the development of lasers and phosphors in lighting applications and as an alternative to quantum dots in the development of photonic and optoelectronic devices. In this contribution we will present a combined ab initio and experimental study of the structural, dynamical and mechanical stability properties of some A$_2$B$_5$O$_{12}$ garnets under high pressure.

12:00PM C3.00004 Towards a Predictive First-Principles Description of High Pressure Hydrogen with Density Functional Theory, MIGUEL A. MORALES, LLNL, JEFFREY M. MCMAHON, UIUC, CARLO PIERLEONI, U. L'Aquila, DAVID M. CEPERLEY, UIUC — We present a study of the influence of the main approximations employed in first-principles descriptions of high pressure hydrogen with Density Functional Theory. We focus on the importance of nuclear quantum effects (NQE) on equilibrium properties of both liquid and solid molecular hydrogen close to dissociation. We find that NQEs strongly influence intramolecular properties, such as bond stability, and are thus an essential part of the dissociation process. In addition, we show how the combination of both thermal and quantum effects make a drastic change to the predicted optical properties of the molecular solid, demonstrating the very limited value of predictions based on classical ions and static crystals. We also focus on the influence of the chosen exchange–correlation density functional on the predicted properties of hydrogen, including the location of the Liquid-Liquid Phase Transition and the pressure dependence of the band gap in the solid.

12:15PM C3.00005 Origin of Metallization of FeO at High Temperatures and Pressures from First-principles DFT-DMFT Computations, R.E. COHEN, Geophysical Lab, Carnegie Institution, KRISTJAN HAULE, Dept. Phys., Rutgers Univ. — Experiments and theory show that FeO metallizes at high temperatures (∼2000K) and pressures (∼80 GPa) [1]. Here we use DFT+Dynamical Mean Field Theory (DMFT) with continuous time quantum Monte Carlo (CTQMC) to study the origin of the metallization. We find with increasing pressure in paramagnetic FeO in a cubic lattice a high-spin low-spin transition, with a wide transition region between characterized by intermediate occupancies of the t2g and eg states between. We find that at 300K cubic FeO remains insulating to a factor of two compression (over 600 GPa), except for a small region of high spin metal. However, at high temperatures (e.g. 2000K) a metallic state is found under compression. The metallization occurs from thermal fluctuations among different multiplets representing high- and low-spin states. We are now studying the AFM ground state, the Néel transition, and (Mg,Fe)O solid solutions. This work is supposed by NSF.


Monday, July 8, 2013 11:00AM - 12:30PM — Session C4 EM.3 Small Scale Safety Testing — Vashon - Daniel Preston, Los Alamos National Laboratory
11:00AM C4.00001 Statistical Evaluation of Small-scale Explosives Testing, CLINT GUYMON, Safety Management Services, Inc. — Small-scale explosives sensitivity testing is used to qualitatively and quantitatively evaluate risk. Both relative comparison and characterization of the transition from no reaction to reaction is used to estimate that risk. Statistical comparisons and use of statistically efficient methods are critical to accurately and efficiently make risk related decisions. Many public and private entities are not making accurate decisions based on the test data because of the lack of properly applying basic statistical principles. We present methods and examples showing how to use statistics to accurately and efficiently evaluate the risk. Some of the methods presented include the Significance Chart Method and adaptive step-size techniques like the Neyer D-Optimal method. These methods are compared to the more traditional approaches like Brueton and Probit. Use of statistical methods can significantly improve the efficiency, accuracy, and applicability of small-scale explosives sensitivity testing.

11:30AM C4.00002 Automated High-Speed Video Detection of Small-Scale Explosives Testing, ROBERT FORD, CLINT GUYMON, Safety Management Services, Inc. — Small-scale explosives sensitivity test data is used to evaluate hazards of processing, handling, transportation, and storage of energetic materials. Accurate test data is critical to implementation of engineering and administrative controls for personnel safety and asset protection. Operator mischaracterization of reactions during testing contributes to either excessive or inadequate safety protocols. Use of equipment and associated algorithms to aid the operator in reaction detection can significantly reduce operator error. Safety Management Services, Inc. has developed an algorithm to evaluate high-speed video images of sparks from an ESD (Electrostatic Discharge) machine to automatically determine whether or not a reaction has taken place. The algorithm with the high-speed camera is termed GoDetect (patent pending). An operator assisted version for friction and impact testing has also been developed where software is used to quickly process and store video of sensitivity testing. We have used this method for sensitivity testing with multiple pieces of equipment. We present the fundamentals of GoDetect and compare it to other methods used for reaction detection.

11:45AM C4.00003 Improved Sensitivity Testing of Explosives Using Transformed Up-Down Methods, GEOFFREY BROWN, Los Alamos National Laboratory — Sensitivity tests provide data that help establish guidelines for the safe handling of explosives. Any sensitivity test is based on assumptions to simplify the method or reduce the number of individual sample evaluations. Two common assumptions that are not satisfied are 1) explosive response is linear in the applied stimulus levels and 2) the chosen test level spacing is close to the standard deviation of the explosive response function (for Brueton Up-Down testing). In this work we present efforts to improve sensitivity testing by addressing these assumptions using Transformed Up-Down (TUD) test methods augmented with simple algorithms. TUD methods have been developed extensively for psychometric testing applications over the past 50 years and generally use multiple tests at a given level to determine whether to increase or decrease the applied stimulus. In the context of our work, we can use TUD methods that concentrate testing around useful probability levels and augment them with algorithms for adjusting test level spacing during the evaluation. Transformed methods that we have developed to address the assumptions noted above will be examined and evaluated with simulation to highlight their properties and assess their usefulness.

12:00PM C4.00004 Department of Homeland Security (DHS) Proficiency Testing on Small-Scale Safety and Thermal Testing of Improvised Explosives, JOHN G. REYNOLDS, LLNL, MARY M. SANDSTROM, GEOFFREY W. BROWN, LANL, KIRSTIN F. WARNER, NSWC-IHD, JASON J. PHILLIPS, SNL, TIMOTHY J. SHELLEY, ATF Huntsville, JOSE A. REYES, ARA Tyndall AFB, PETER C. HSU, LLNL — One of the first steps in establishing safe handling procedures for explosives is small-scale safety and thermal (SSST) testing. To better understand the response of improvised materials or HMEs to SSST testing, 18 HME materials were compared to 3 standard military explosives in a proficiency-type round robin study among five laboratories—2 DoD and 3 DOE—sponsored by DHS. The testing matrix has been designed to address problems encountered with improvised materials—powder mixtures, liquid suspensions, partially wetted solids, immiscible liquids, and reactive materials. Over 30 issues have been identified that indicate standard test methods may require modification when applied to HMEs to derive accurate sensitivity assessments needed for development safe handling and storage practices. This presentation will discuss experimental difficulties encountered when testing these problematic samples, show inter-laboratory testing results, show some statistical interpretation of the results, and highlight some of the testing issues.

3 Some of the work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-017519 (721812).

12:15PM C4.00005 Safety Testing of Ammonium Nitrate Based Mixtures, JASON PHILLIPS, KARMEN LAPPO, JAMES PHELAN, NATHAN PETERSON, DON GILBERT, Sandia National Laboratories — Ammonium nitrate (AN)/ammonium nitrate based explosives have a lengthy documented history of use by adversaries in acts of terror. While historical research has been conducted on AN-based explosive mixtures, it has primarily focused on detonation performance while varying the oxygen balance between the oxidizer and fuel components. Similarly, historical safety data on these materials is often lacking in pertinent details such as specific fuel type, particle size parameters, oxidizer form, etc. A variety of AN-based fuel-oxidizer mixtures were tested for small-scale sensitivity in preparation for large-scale testing. Current efforts focus on maintaining a zero oxygen-balance (a stoichiometric ratio for active chemical participants) while varying factors such as charge geometry, oxidizer form, particle size, and inert diluent ratios. Small-scale safety testing was conducted on various mixtures and fuels. It was found that ESD sensitivity is significantly affected by particle size, while this is less so for impact and friction. Thermal testing is in progress to evaluate hazards that may be experienced during large-scale testing.

Monday, July 8, 2013 11:00AM - 12:30PM — Session C5 GP1: Geophysics

11:00AM C5.00001 Phase relations of Earth’s core materials, TETSUYA KOMABAYASHI, Department of Earth and Planetary Sciences, Tokyo Institute of Technology — Knowledge of thermodynamic state of the Earth’s core is of primary importance for understanding the evolution of the solid Earth. In addition to iron which is its major component, several amounts of nickel and light element(s) should also be present in the core. I will review phase relations of these systems from recent high-pressure (P) and temperature (T) experiments and thermodynamic modeling. First, I will introduce recent technical development of the so-called resistive internally heated diamond anvil cell (DAC) experiments in which thin iron (alloy) foil serves as a heater and a sample simultaneously. By resistance heating, it produces much more stable heating than the laser-heating technique and much higher temperature than the external-heating system. With this technique we conducted high-P-T in-situ measurements of the gamma-epsilon transitions in Fe and Fe-Ni alloy. In addition, I will also present new data of phase relations of Fe-Si alloy for which consistent phase relations have not been established so far. Next, thermodynamics of the core materials will be discussed based on the latest static high-P-T experiments. I constructed a thermodynamic model of melting relations in the system Fe-FeO to the outer core inner core boundary (ICB) pressure. At the ICB pressure, calculations assuming the ideal solution for liquids show that the eutectic temperatures are much lower than results of DAC experiments showing a solid assemblage Fe-FeO at the same P-T conditions. Then, non-ideality of mixing for liquids was assessed to make the eutectic temperature consistent with the experiments. With the new solution model, the eutectic compositions under the core pressures are calculated. From the Gibbs free energy for the Fe-FeO liquids, I calculate the density, sound velocity, and adiabatic temperature profile of a hypothetical oxygen-bearing outer core. On the basis of these results, I will discuss if oxygen can be a major light element in the core or not.
11:30AM C5.00002 Gas recovery experiments to determine the degree of shock-induced devolatilization of calcite. SOHSUKE OHNO, KO I SHIBASHI, Planetary Exploration Research Center / Chiba Institute of Technology, TOSHIMORI SEKINE, Hiroshima University, KOSUKE KUROSAWA, Japan Aerospace Exploration Agency, TAKAMICHI KOBAYASHI, National Institute for Material Science, SEIJI SUGITA, University of Tokyo, TAKAFUMI MATSUI, Planetary Exploration Research Center / Chiba Institute of Technology — Shock-induced devolatilization of volatile-bearing minerals has played important roles in formation of the atmosphere and the evolution of surface environments of terrestrial planets. The dependence of the degree of devolatilization on the ambient pressure have not detailedly investigated before, although the ambient pressure must dramatically change the degree of devolatilization. In this study, we conducted shock-recovery experiments of calcite (CaCO₃) using newly designed sample containers for released gas analysis and assess the dependence of the degree of devolatilization on the ambient pressure. The results clearly shows that the degree of devolatilization increases as the sample container volume increases and the initial mass of calcite decreases.

11:45AM C5.00003 Electrical Resistivity of natural Marcasite at High-pressures¹, GOPALAKRISHNARAO PARTHASARATHY, CSIR-National Geophysical Research Institute, Hyderabad, 500007, India — Marcasite is considered to be a common iron sulfide in reducing Martian sediments and may enclose microbial remains during growth and hence study of marcassite may have significance in the search for fossil life on Mars. The high-pressure phase stability investigations of marcassite are useful in understanding the sulfide mineralogy of Martian surface, affected by meteorite impacts. The sulfides were characterized by electron microprobe micro analyses (EPMA), powder X-ray diffraction, DTA, and FTIR spectroscopic measurements. The samples were powdered by a porcelain mortar and pestle. The chemical composition of the sample was determined by an electron probe micro-analyzer (EPMA). High-pressure electrical resistivity measurements were carried out on natural marcassite, and marcassite rich samples (Marcasite 95 mol % pyrite 5 mol % ) up to 7 GPa. Marcasite sample shows a discontinuous decrease in the electrical resistivity at 5. 2 (± 0.5) GPa indicating a first order phase transition. The Differential thermal analyses and the Fourier transform infrared spectroscopic measurements on the pressure quenched sample shows the characteristics of pyrite, indicating the pressure induced marcassite-to-pyrite transition of the natural marcassite at 5. 2 (± 0.5) GPa. The observation of marcassite to pyrite phase transition may be useful in estimating the pressure experienced by shock events on the Martian surface as well as the meteorites where marcassite-pyrite phases coexist.

¹Financial support from CSIR-SHORE-PSC0205

12:00PM C5.00004 On the Composition and Temperature of the Terrestrial Planetary Core¹, YANGWEI FEI, Carnegie Institution of Washington — The existence of liquid cores of terrestrial planets such as the Earth, Mars, and Mercury has been supported by various observation. The liquid state of the core provides a unique opportunity for us to estimate the temperature of the core if we know the melting temperature of the core materials at core pressure. Dynamic compression by shock wave, laser-heating in diamond-anvil cell, and resistance-heating in the multi-anvil device can melt core materials over a wide pressure range. There have been significant advances in both dynamic and static experimental techniques and characterization tool. In this talk, I will review some of the recent advances and results relevant to the composition and thermal state of the terrestrial core. I will also present new development to analyze the quenched samples recovered from laser-heating diamond-anvil cell experiments using combination of focused ion beam milling, high-resolution SEM imaging, and quantitative chemical analysis. With precision milling of the laser-heating spo, the melting point and element partitioning between solid and liquid can be precisely determined. It is also possible to re-construct 3D image of the laser-heating spot at multi-megabar pressures to better constrain melting point and understanding melting process. The new techniques allow us to extend precise measurements of melting relations to core pressures, providing better constraint on the temperature of the core.

¹The research is supported by NASA and NSF grants.

Monday, July 8, 2013 11:00AM - 12:30PM  Session C6 ME.1 Particulate/Porous Materials II  Cascade II - John Borg, Marquette University

11:00AM C6.00001 Criticality of damage-failure transitions under dynamic and shock wave loading¹, OLEG NAIMARK, Institute of Continuous Media Mechanics RAS — Specific type of criticality in defect ensembles — structural-scaling transition related to damage-failure scenarios under dynamic and shock wave loading was established. It allowed development of phenomenology of damage-failure transition induced by defects collective modes, supported by experiments and high resolution “in-situ” study of dynamic crack propagation and spall failure in PMMA and vanadium, dynamic fragmentation statistics in glass and ceramics. Structural (SWFM and AFM) study in terms of scaling invariance established the linkage of evolution of these modes with material responses in large range of load intensity and interpretation of the links of dynamic crack branching and specific morphology of numerous spall failure in PMMA, multiscale invariance in defect ensembles as spall failure precursor in shocked vanadium, 1/f flicker noise statistics of fragmentation according to the temporal analysis of fracture luminescence data in fused glass and zirconium dioxide shocked bars. Simulation of mentioned experiments supported the features of universality related to the self-similar solution of collective modes of defects in the course of structural-scaling transition.

¹Research was supported by projects RAS 12-1-1021, 12-1-12; RFBR 11-01-00712

11:15AM C6.00002 Shock Hugoniot Measurements in Foam OREN PETEL, McGill University, Department of Mechanical Engineering, Montréal, QC, H3A 0C3, Canada, SIMON OUELLET, Defence Research and Development Canada Valcartier, Québec, QC, G3J 1X5, Canada, DAVID FROST, ANDREW HIGGINS, McGill University, Department of Mechanical Engineering, Montréal, QC, H3A 0C3, Canada — Foams are found in a variety of process requirements. In industrial applications, foams are exposed to shock wave loadings, there is a considerable lack of shock Hugoniot data for these materials. Typical characteristics of foams have involved the use of split-Hopkinson pressure bars or quasi-static compression machines to determine the stress-strain relationship in the foams. As such, the elastic-plastic response of foam at intermediate pressure ranges continues to be a source of confusion. In the present study, Photonic Doppler Velocimetry is used to measure the shock Hugoniot of a foam for a comparison to its quasi-static compression curves. The deviation of these two curves will be discussed and compared to common plasticity models used to describe dynamic foam behaviour in the literature.

11:30AM C6.00003 Modeling of laser-driven shocks into porous graphite GABRIEL SEISSON, DAVID HÉBERT, ISABELLE BERTRON, CEA CESTA, CS00001, 33116 Le Barp Cedex, France, LAURENT VIDEAU, PATRICK COMBIS, CEA DIF, 91297 Arpajon, France, LAURENT BERTHE, Laboratoire PIMM UPR8006, 151 bd de l‘Hôpital, 75013 Paris, France, MICHEL BOUSTIE, Institut PPRIME UPR3346, 1 av Clémence Adler, 86961 Futuroscope Cedex, France — This paper presents experiments of laser-driven shocks into a commercial grade of porous graphite. Intensities of about 3 GW.cm⁻² led to pressures close to 3 GPA on the front surfaces of the 0.5 mm samples. The rear surface velocities, recorded by a Velocity Interferometer System (VISAR), ranged from 250 to 325 m.s⁻¹. Two classical models for porous materials are discussed. The first one uses plates of dense graphite spaced out in order to obtain the correct average density. The second one models a continuous material and includes an experimental compaction curve of our porous graphite. They were implemented into hydrocodes and both gave quite correct maximum free surface velocities and shock break-out instants. Nevertheless, the continuous representation appeared to be more efficient to reproduce the experimental free surface velocity ramp. Discussions on the laser-matter interaction modeling are also provided. Finally, a protocol for the simulation of future laser experiments is proposed.
11:45AM C6.00004 Mesoscale Simulations of the Shock and Release of an Aluminum-Polymer System
JOHN BORG, Marquette University, RUSS MAINES, Eglin Air Force Base, RAYMOND RYCKMAN, Jacobs Technology, Inc. TEAS Group, LALIT CHHABILDA, Eglin Air Force Base — Fundamental questions remain in developing a more complete understanding of the dynamic behavior of heterogeneous materials; the development of which is complicated by a lack of experimental data at the mesoscale. Whereas experiments measure the bulk response, mesoscale simulations facilitate a more complete understanding of the system’s response. In this work mesoscale simulations were used to explore the dynamic response of aluminum foam filled with polyvinylidene fluoride (PVDF) over a range of impact velocities from 350 to 2220 m/s (20 GPa). The results are compared to experiments. The simulated bulk Hugoniot states agree with experiments, the distribution of stress and temperature along the Hugoniot will be presented. The release paths however are more sensitive to the polymer’s equation of state (EOS). Like other polymers, PVDF exhibits a variety of complicated responses including a non-linear shock velocity-particle velocity Hugoniot especially at low particle velocities, a low melt temperature, a polymorphic phase transformation near 30 GPa and possibly an increase in the Grueneisen parameter with an increase in density. An EOS for PVDF that includes all of these phenomena was constructed; the result improved the simulated release paths when compared to the experimentally measured release paths. The effect of each phenomena on the shock and release will be presented; the Grueneisen parameter had the strongest affect on release.

12:00PM C6.00005 Shock Propagation Modeling in Heterogeneous Materials THOMAS A. HAIL, Sandia National Laboratories — Shock compression of foams is an intriguing research area that challenges our abilities to model experiments using computer simulations that span 9 orders of magnitude in spatial scales from the atomistic scale through the mesoscale and up to the continuum levels. Experiments test shock compression of dense polymers, polymer foams, and high-Z doped foams. Random distributions of polymer fibers, variations in pore size, and non-uniformities in the bulk properties of the foam (such as mean density) lead to spread in the experimental data. Adding dopants to foams introduces new complexities and the effect of the distribution and sizes of dopant particles must be characterized and understood. Therefore we turn to computer simulation to illuminate the intricacies of the experiments that cannot be directly measured. This paper overviews of our range of methods to model pure and platinum-doped poly-methyl-entene (PMP) foams. At the nanometer scale, hydrodynamic simulations compare favorably to classical molecular dynamics (MD) simulations of porous foams, verifying models of foam vaporization under strong shock conditions. Inhomogeneous mesoscale and homogenized continuum simulations present contrasting pictures of shocked foams. Mesoscale simulations at the micron scale have diffuse shock widths that depend upon the pore size, and post-shock vorticity results in fluctuations about the mean post-shock state and lower mean pressures and temperatures. Homogenized simulations, in the limit of zero pore size, have nanoscale shock widths, steady shock-shock states, and higher mean pressures and temperature that compare favorably with 1D analysis of experiments. We reconcile the contrasting mesoscale and continuum views using theoretical turbulent corrections to the Hugoniot jump condition to show a consistent picture of shocked foams over 9 orders of spatial scale.

VICTORIA STOLYAR, GURUSWAMI RAVICHANDRAN, California Institute of Technology, SCOTT ALEXANDER, Sandia National Laboratories — At high pressures, and high strain rates, the measurement of strength is important to many implications including planetary impact and inertial confinement fusion. Understanding how strength depends on pressure allows for the characterization of materials and validation of constitutive models. Slotted barrel guns have traditionally been used in experiments, such as the pressure-plate impact technique, to generate longitudinal and shear waves through an oblique impact. A new methodology for measuring material strength using normal impact (1-2km/s) is described. In this configuration, a composite target is designed with an angled material of interest embedded into a driver material. This driver material is used to generate an oblique shock wave that is followed by a shear wave, due to the angled nature of the target material. Using shock polar analysis, the rear surface of the target is designed to be parallel to the transmitted shock wave in order to mitigate wave interactions at the rear surface. A window is used on the rear surface of the target to measure the in-situ particle velocities at the target-window interface. Using three VISAR measurements, the tangential and longitudinal particle velocities at the rear surface of the target are found from which the shear stress (strength) is inferred as a function of pressure. Results are presented for 6061-T6 Aluminum as well as Tantalum. Hydrocode simulations are used to predict the experimental results as well as characterize the wave interactions in the oblique wedge experiments.

Monday, July 8, 2013 1:45PM - 3:15PM — Session D1 ME.4 Strength III
Grand Ballroom I - Adam Schwartz, Lawrence Livermore National Laboratory

2:45PM D1.00001 Oblique Plate Impact Experiments to Study the Compression-Shear Behavior of the HMX Based Explosive PBX 9501 WILLIAM REINHART, Sandia National Laboratories, RICK GUSTAVSEN, Los Alamos National Laboratory, TRACY VOGLER, SCOTT ALEXANDER, Sandia National Laboratories, TOM THORNHILL, Ktech-Raytheon, BRAD CLEMENTS, BRIAN BARTRAM, Los Alamos National Laboratory, SNL/LANL COLLABORATION — HMX (cyclotetramethylene-tetranitramine) based explosive, PBX 9501, is a conventional high explosive formulation composed of 95% wt. of HMX and 5% binders. A series of experiments were performed to investigate one-dimensional combined pressure-shear wave transmission in PBX-9501. This study is thought to be the first to estimate shock stress and strength in a plastic bonded high explosive. Experiments were conducted using Sandia National Laboratories oblique launcher at the Shock Thermodynamics Applied Research (STAR) facility. A projectile is keyed to a slot in the launcher barrel in order to prevent rotation. The projectile is faced with a titanium alloy plate inclined at 20 degrees to the launcher axis. The target consists of a 1 mm thick PBX 9501 disk sandwiched between two titanium alloy plates. Measurements of shear and longitudinal particle velocities were used to determine stresses and infer strength. Longitudinal stresses from 1.4 to 3.1 GPa were applied which presented corresponding shear stresses of 0.1 to 0.23 GPa at high shearing strain rates up to 0.4 x 10^6 s^-1. This experimental data now provides for the first time, relevant information for model development.

2:00PM D1.00002 Measurement of Strength at High Pressures Using Oblique Shock Waves VICTORIA STOLYAR, GURUSWAMI RAVICHANDRAN, California Institute of Technology, SCOTT ALEXANDER, Sandia National Laboratories — High pressures and high strain rates, the measurement of strength is important to many implications including planetary impact and inertial confinement fusion. Understanding how strength depends on pressure allows for the characterization of materials and validation of constitutive models. Slotted barrel guns have traditionally been used in experiments, such as the pressure-plate impact technique, to generate longitudinal and shear waves through an oblique impact. A new methodology for measuring material strength using normal impact (1-2km/s) is described. In this configuration, a composite target is designed with an angled material of interest embedded into a driver material. This driver material is used to generate an oblique shock wave that is followed by a shear wave, due to the angled nature of the target material. Using shock polar analysis, the rear surface of the target is designed to be parallel to the transmitted shock wave in order to mitigate wave interactions at the rear surface. A window is used on the rear surface of the target to measure the in-situ particle velocities at the target-window interface. Using three VISAR measurements, the tangential and longitudinal particle velocities at the rear surface of the target are found from which the shear stress (strength) is inferred as a function of pressure. Results are presented for 6061-T6 Aluminum as well as Tantalum. Hydrocode simulations are used to predict the experimental results as well as characterize the wave interactions in the oblique wedge experiments.

2:15PM D1.00003 ABSTRACT WITHDRAWN

2:45PM D1.00004 Measurement of dynamic strength at high pressures using magnetically applied pressure-shear (MAPS) on the Sandia Z accelerator C.S. ALEXANDER, T.A. HAIL, D.G. DALTON, D.C. ROVANG, D.C. LAMPPA, Sandia National Laboratories — The recently developed magnetically applied pressure-shear (MAPS) technique used to measure dynamic material strength at high pressures on magneto-hydrodynamic (MHD) drive pulsed power platforms has been implemented on the Sandia Z accelerator. MAPS relies on an external magnetic field normal to the plane of the MHD drive current to directly induce a shear stress wave in addition to the usual longitudinal stress wave. This shear wave is used to directly probe the strength of a sample. By implementing this technique on Z, far greater pressures can be attained than were previously available using other MHD facilities. In addition, the use of isentropic compression will limit sample heating allowing the measurement to be made at a much lower temperature than under shock compression. Details of the experimental approach, including design considerations and analysis of the results, will be presented along with the results of Z experiments measuring the strength of tantalum at pressures up to 50 GPa, a five-fold increase in pressure over previous results using this technique.
3:00PM D1.00005 Shock compression of pyrolytic graphite to 18 GPa: Effect of orientational order, M. LUCAS, J.M. WINEY, Y.M. GUPTA, Washington State University — Wave profiles for highly-oriented pyrolytic graphite (HOPG) shocked above the onset stress for phase transformation (~20 GPa) depend strongly on the HOPG orientational order [Erskine and Nellis, Nature 349, 317 (1991)]. To gain insight into this finding, the shock responses for three pyrolytic graphites, differing in their orientational order, are compared for peak stresses below the onset for phase transformation. Measured wave profiles reveal significant differences in the elastic-inelastic response of: (from most to least oriented) ZYB-grade HOPG, ZYH-grade HOPG, and as-deposited pyrolytic graphite (PG). For peak stresses above 9 GPa, ZYB-grade HOPG exhibits elastic-inelastic wave profiles with large elastic wave amplitudes. The elastic wave amplitude increases linearly with peak stress, reaching 16 GPa for a peak stress of 18 GPa. In contrast, overdriven waves for ZYH-grade HOPG and PG suggest negligible elastic limits. Measured peak states indicate that PG is more compressible than ZYB- and ZYH-grade HOPG. These differences indicate that the elastic-inelastic response of shocked pyrolytic graphite depends strongly on the orientational order, and this dependence will likely persist to peak stresses approaching the phase transformation onset. Work supported by DOE/NNSA.

Monday, July 8, 2013 1:45PM - 3:15PM –
Session D2 CM.2 Phase Transitions: Quantum & Topological
Grand Ballroom II - Frank Cherne, Los Alamos National Laboratory

1:45PM D2.00001 Quantum Criticality and Superconductivity in Spin and Charge Systems.
SIDDHARTH SAXENA, Cambridge University — This talk will focus on experimental search and discovery of novel forms of quantum order in metallic and insulating magnets, intercalated compounds, ferroelectric systems and multi-ferroic materials. Particularly discussed will be the pressure-induced superconductivity and critical phenomena in the vicinity of quantum phase transitions. Materials tuned to the neighbourhood of a zero temperature phase transition often show the emergence of novel quantum phenomena. Much of the effort to study these new emergent effects, like the breakdown of the conventional Fermi-liquid theory in metals has been focused in narrow band electronic systems. But Spin or Charge ordered phases in insulating systems can also be tuned to absolute zero using hydrostatic pressure. Close to such a zero temperature phase transition, physical quantities like resistivity, magnetisation and dielectrics constant change into radically unconventional forms due to the fluctuations experienced in this region giving rise to new kinds ordered states including superconductivity in the metallic systems

2:15PM D2.00002 Pressure-induced quantum critical behavior in the heavy-fermion compound CeCoGe$_{2}$Si$_{1-x}$Si$_{x}$, J. LARREA JIMENEZ, M. MARTELLI, S. PASCHEN, Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria, J. TEYSSIER, Département de Physique de la Matière Condensée, Université de Genève, Switzerland, A. STRYDOM, University of Johannesburg, H. RONNOW, Laboratory for Quantum Magnetism, École Polytechnique Fédérale de Lausanne, Switzerland — The pressure-tuned quantum critical point (QCP) of the antiferromagnetic heavy-fermion compound CeCoGe$_{2}$Si$_{1-x}$Si$_{x}$ was claimed to be dominated by different effects on both sides of the QCP: on the magnetic side spin fluctuations govern the criticality, while on the non-magnetic side the criticality is dominated by disorder that quenches the spin fluctuations. Here we study high-quality CeCoGe$_{2}$Si$_{0.8}$ samples with residual resistance ratios four times larger than those of the previously investigated CeCoGe$_{2}$Si$_{0.9}$ samples. Interestingly, while DC magnetic susceptibility measurements show that the Néel temperature of $T_N = 4K$ at zero pressure is only slightly reduced by pressure up to 3.0 kbar, a much stronger decrease is observed for the specific heat anomaly. We will present electrical resistivity and specific heat measurements up to 15 kbar and down to 0.05 K, and establish the pressure – temperature phase diagram for CeCoGe$_{2}$Si$_{0.5}$. The critical behavior shall be compared to the one observed for both CeCoGe$_{2}$Si$_{0.9}$ and the pure reference compound CeCoGe$_{1}$.

2:30PM D2.00003 Pressure induced phase transitions studies using advanced synchrotron techniques, HAOZHE LIU, LISA LIU, JINGGENG ZHAO, Harbin Institute of Technology, HIT OVERSEAS COLLABORATIVE BASE AT ARGONNE COLLABORATION — In this presentation, the joint effort on high pressure research through program of Harbin Institute of Technology (HIT) Overseas Collaborative Base at Argonne will be introduced. Selected research projects on pressure induced phase transitions at room temperature and high/low temperature conditions, such as A2B3 type topological insulators, iron arsenide superconductors, piezoelectric/ferroelectric materials, ABO3 type single crystals and metallic glasses, will be presented. Recent development on imaging and diffraction tomography techniques in diamond anvil cell will be reviewed as well.

2:45PM D2.00004 ABSTRACT WITHDRAWN –

Monday, July 8, 2013 1:45PM - 3:15PM –
Session D3 NT.1 Novel Techniques: Flyers and Guns
Fifth Avenue - Anthony Fredenburg, Los Alamos National Laboratory

1:45PM D3.00001 Development of an accelerating-piston implosion-driven launcher, JUSTIN HUNEAULT, JASON LOISEAU, ANDREW HIGGINS, McGill University — The ability to soft-launch projectiles at velocities exceeding 10 km/s is of interest to several scientific fields, including orbital debris impact testing and equation of state research. Current soft-launch technologies have reached a performance plateau below this operating range. The energy and power density of high explosives provides a possible avenue to reach this velocity if used to dynamically compress a light driver gas to significantly higher pressures and temperatures compared to light-gas guns. In the implosion-driven launcher (IDL), linear implosion of a pressurized tube drives a strong shock into the gas ahead of the tube pinch, thereby forming an increasingly long column of compressed gas which can be used to propel a projectile. The McGill IDL has demonstrated the ability to launch a 0.1-g projectile to 9.1 km/s. This study focuses on the implementation of a novel launch cycle wherein the explosively driven pinch is accelerated down the length of the tube in order to maintain a relatively constant projectile base pressure early in the launch cycle. The experimental development of an accelerating driver which utilizes an explosive lens to phase the detonation wave is presented. The design and experimental performance of an accelerating-piston IDL is also discussed.
A highlight of the new capability along with discussion of the initial experiments to date will be presented including future areas of research. Future experiments to evaluate the safety of new explosive formulations to bullet impactors.

2:30PM D3.00004 Ramp Wave Generation Using Graded Areal Density Ceramic Flyers and the Plate Impact Technique, PETER TAYLOR, AWE, GARETH APPLEBY-THOMAS, MICHAEL GOFF, Cranfield University, PAUL HAZELL, University of New South Wales, JAMES LEIGHS, DAVID WOOD, Cranfield University — Ramping shock waves of the order of 2.4 GPa were generated in Kel-F targets through the use of graded areal density ceramic flyers via the gas gun plate impact technique, with a buffer disc employed between the flyer and the target to eliminate penetration by the ceramic flyer. Ramp wave parameters were varied through alteration of the areal density gradient and the thickness of the buffer disc used. Observations of the ramped shock were undertaken through the use of embedded particle velocity gauges and the results compared with hydrocode calculations. The discussion of results includes details of the magnitude, gradient, and planarity of the ramp waves produced at various positions in the target material. The flyers were fabricated from alumina ceramic with the ceramic laser stereo-lithography process. In order to characterise the material for modelling purposes a series of shots were carried out to compare the Hugoniot of this material with conventionally sintered material, these results are presented.

3:00PM D3.00006 Modelling the Equation of State of a Graded Density Impactor, GEOFFREY COX, JOHN MAW, AWE — There is a requirement for off-Hugoniot data to validate material models. One technique is to use projectiles with graded shock impedance layers in a gas gun to impact a target and apply a ramp loading. To accurately design a shock profile to be applied to the target the impactor should be modelled. This also provides an assessment of whether lateral rarefactions will hinder the experiment, and increases confidence in the analysis of the results obtained. This talk considers several methods for calculating the equation of state of particulate mixtures for application to the modelling of graded density impactors.


1:45PM D4.00001 ABSTRACT WITHDRAWN –

2:00PM D4.00002 Bullet Impact Safety Study of PBX-95021, LOUIS FERRANTI, Lawrence Livermore National Laboratory — A new small arms capability for performing bullet impact testing into energetic materials has recently been activated at Lawrence Livermore National Laboratory located in the High Explosives Applications Facility (HEAF). The initial capability includes 0.223, 0.30, and 0.50 testing calibers with the flexibility to add other barrels in the near future. An initial test series has been performed using the 0.50 caliber barrel shooting bullets into targets using the TATB based explosive PBX-9502 and shows an expected non-violent reaction. Future experiments to evaluate the safety of new explosive formulations to bullet impact are planned. A highlight of the new capability along with discussion of the initial experiments to date will be presented including future areas of research.

1This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
2:15PM D4.00003 Size-effect of explosive sensitivity under low velocity impact

DANZHU MA, PENGWAN CHEN, QIANG ZHOU, Beijing Institute of Technology — Low velocity impact may ignite the solid high explosives and cause undesired explosion incidents. The safety of high explosives under low velocity impact is one of the most important problems in handling, manufacture, storage, and transportation procedures. More and more high-velocity impact tests have been developed for low velocity impact scenarios, including but not limited to the drop hammer impact test, the Susan test, the Spigot test, and the Steven test, with a charge mass varying from tens of milligrams to several kilograms. The effects of specimen size on explosive sensitivity were found in our drop hammer impact test and Steven tests, including the threshold velocity/height and reaction violence. To further analyze the size effects on explosive sensitivity under low velocity impacts, we collected the impact sensitivity data of several PBX explosives in the drop hammer test, the Steven test, the Susan test and the Spigot test. The effective volume of explosive charge and the threshold specific mechanical energy were introduced to investigate the size-effect on the explosive ignition thresholds. The effective volume of explosive charge in Steven test and Spigot test were obtained by numerical simulation, due to the localization of the impact. The threshold specific mechanical energy is closely related to the effective volume of explosive charge. The results show that, with the increase of effective volume, the specific mechanical energy needed for explosive ignition decreases and trends to reach a constant value. The mechanisms of size effects on explosive sensitivity are also discussed.

2:30PM D4.00004 Microscopic modeling of ignition and burning for well-arranged energetic crystals in response to drop-weight impact

YANQING WU, FENGLEI HUANG, State key Laboratory of Explosion Science and Technology, Beijing Institute of Technology — It has long been recognized that during impact of energetic crystalline solids, some form of energy localization must focus the impact energy into hot spots. However, it was insufficient to obtain just the energy required to cause ignition of an individual hot spot. Hot-spots ignition as well as the subsequent burning together determines the possible occurrence of explosion. A micromechanics theoretical approach was developed, to model hot-spots formation and growth for burning of a single layer of impacted energetic particles. To provide supporting evidence for theoretical analyses, numerical simulations were performed to investigate the thermo-mechanical interactions among the well-arranged energetic crystals. Once hot-spots ignition occurs, the macrokinetics of chemical reactions can be determined by hot-spots density, combustion wave velocity and geometric factor. Considering the micro-particle plasticity, frictional heating, melting, fracture, and chemical reaction at particle level, effects of loading parameters and sample characteristics on ignition and burning were discussed. The resulting reaction may or may not develop into a violent event, which is highly related to the combustion velocity characteristics. Above this frequency, the active heating mechanisms are likely related to particle-scale processes. The observed phenomena may prove useful in the aid of current trace vapor detection methods for explosives.

3:00PM D4.00006 The ODTX System for the Study of Thermal Sensitivity and Thermal Explosion Violence of Energetic Materials

PETER HSU, GARY HUST, JOHN REYNOLDS, KEO SPRINGER, LARRY FRIED, JON MAIENSCHIN, Lawrence Livermore National Laboratory — Incidents caused by fire and combat operations in battlefields can expose energetic materials to unheated heat that may cause thermal explosion, structural damage and casualty. Some explosives may thermally explode at low temperatures (< 100 C) and the violence from thermal explosion may cause a significant damage. Thus it is important to understand the response of energetic materials to thermal insults. The One Dimensional Time to Explosion (ODTX) system at the Lawrence Livermore National Laboratory can measure times to explosion, threshold thermal explosion temperature, and determine kinetic parameters of energetic materials. Samples of different configurations (pressed part, powder, paste, and liquid) can be tested in the system. The ODTX testing can also provide useful data for assessing the thermal explosion violence of energetic materials. In this paper, we will present some recent ODTX experimental data and compare thermal explosion violence of different energetic materials.

Monday, July 8, 2013 1:45PM - 3:15PM — Session D5 EM.2 Shock to Detonation I

1:45PM D5.00001 Discrete effects in energetic materials

ANDREW HIGGINS, McGill University — The classical theory of detonation wave propagation has been highly successful in prediction of detonation dynamics based on a macroscopic, continuum-based approach, wherein the heterogeneity of the energetic material only enters the model via the reaction rate term (e.g., hot-spot based reaction mechanisms). The effects of spatial heterogeneity are rarely treated explicitly in detonation models. However, considerable evidence can be found that mesoscale phenomenon can influence the dynamics of the detonation front on scales larger than the heterogeneities. This evidence is critically reviewed, and possible directions for modeling approaches that incorporate the spatial granularity (discreteness) of the energetic material are suggested.

2:15PM D5.00002 Transverse Initiation of an Insensitive Explosive in a Layered Slab Geometry

ERIC K. ANDERSON, TARIQ D. ASLAM, SCOTT T. JACKSON, Los Alamos National Laboratory — Experiments are presented that explore the shock initiating layer dynamics in an insensitive high explosive. Tests were conducted with a PBX 9502 slab bonded on one side to a PBX 9501 slab. For each test, a planar detonation in the PBX 9501 was generated to drive a shock into the PBX 9502. The thickness of the PBX 9501 layer was varied to control the strength and duration of the transmitted shock. Phase velocities at the explosive outer surfaces, wave-front breakout shapes, and post-shock particle velocity histories associated with the detonating and initiating zones in the two explosives are reported and discussed.
behavior observed in distended systems. Experimental methods for obtaining reliable experimental Hugoniot data as well as attempt to describe the physical mechanisms responsible for anomalous where historical Hugoniot data is fraught with difficulty leading to unreliable data or extremely large associated errors. This presentation will present new DENNIS-KOLLER, R. JASON SCHARFF, D. ANTHONY FREDENBURG, Los Alamos National Laboratory — Porous/granular materials are a class of materials of generated fragments based on the loading conditions. Funding was provided by ONR MURI N00014-07-1-0740 (Program Officer Dr. Clifford Bedford) an insight into this clustering behavior. Understanding of the mesoscale mechanisms may be useful to generate more efficient mesostructures and tailor the size for fragments to be composed of a cluster of Al and W particles with little plastic deformation in the interior Al. Hydrocode simulations were conducted to gain VITALI NESTERENKO, University of California, San Diego — Al oxidation has a potential energy release nearly 5 times that of traditional high explosives; explosive testing of Al-W granular composite rings can be used to predict the levels of load (stress) required cause debonding in different geometries. A simple geometry of interest is that of spherical-caps of the filler particles to calculate the so-called Thermodynamic Work of Adhesion that exists between the matrix and filler particles. This under-pinning quantity transition conditions is the magnitude of adhesion that exists between the polymeric matrix binder-system and the filler particles. Experimental measurements of the free surface energies of a number of binders have been made using the Wilhelmy Plate Technique. These data can be combined with equivalent data on the filler particles to calculate the so-called Thermodynamic Work of Adhesion that exists between the matrix and filler particles. This under-pinning quantity can be used to predict the levels of load (stress) required cause debonding in different geometries. A simple geometry of interest is that of spherical-caps of polymers debonding from metal substrates (Al/W). Experiments using this geometry have been performed with an Atomic Force Microscope pull-off technique to measure the critical loads (stresses) required for debonding. There is good agreement between the predicted values based on the Wilhelmy Plate data, and the measured values from the Atomic Force Microscope. Such understanding and experimental data are required for the development and validation of microstructural models for predicting mechanical behaviour over the whole life cycle.

Monday, July 8, 2013 1:45PM - 3:15PM – Session D6 ME.I Particulate/Porous Materials III Cascade II - Darcie Dennis-Koller, Los Alamos National Laboratory

1:45PM D6.00001 Thermodynamic Work of Adhesion measurements of Polymer Bonded eXplosive constituents via the Wilhelmy Plate technique and their application to Atomic Force Microscope pull-off experiments, DAVID WILLIAMSON, NEIL HAMILTON, STEWART PALMER, ANDREW JARDINE, University of Cambridge, CLAIRE LEPPARD, AWE — There is much evidence that the major strength limiting factor for Polymer Bonded eXplosives above their glass-transition condition is the magnitude of adhesion that exists between the polymeric matrix binder-system and the filler particles. Experimental measurements of the free surface energies of a number of binders have been made using the Wilhelmy Plate Technique. These data can be combined with equivalent data on the filler particles to calculate the so-called Thermodynamic Work of Adhesion that exists between the matrix and filler particles. This under-pinning quantity can be used to predict the levels of load (stress) required cause debonding in different geometries. A simple geometry of interest is that of spherical-caps of polymers debonding from metal substrates (Al/W). Experiments using this geometry have been performed with an Atomic Force Microscope pull-off technique to measure the critical loads (stresses) required for debonding. There is good agreement between the predicted values based on the Wilhelmy Plate data, and the measured values from the Atomic Force Microscope. Such understanding and experimental data are required for the development and validation of microstructural models for predicting mechanical behaviour over the whole life cycle.

2:00PM D6.00002 Mechanisms of fragmentation and microstructure of debris generated during explosive testing of Al-W granular composite rings, PO-HSUN CHIU, KARL OLNLEY, University of California, San Diego, CHRIS BRAITHWAITE, ANDREW JARDINE, ADAM COLLINS, GREGORY FRITZ, ADAM STOVER, Cavendish Laboratory, Cambridge, DAVID BENSON, VITALI NESTERENKO, University of California, San Diego — Al oxidation has a potential energy release nearly 5 times that of traditional high explosives; however, the oxidation rate scales with the Al particle size. To oxidize on a time scale of ~1ms, Al particle size needs to be on the order of 20 microns. Highly heterogeneous materials with constituents having drastically different densities and shock impedances (e.g., Al and W) may provide additional mesoscale mechanisms to pulverize the material into much smaller fragments. Explosively driven expanding ring experiments were conducted with Al-W granular composite rings with different morphologies (axial/elongated particles of W, bonded/unbonded Al particles processed using cold and hot isostatic pressing). Recovered fragments showed a significantly reduced fragment sizes compared to a homogeneous sample. Examination of the fragments using SEM showed a propensity for fragments to be composed of a cluster of Al and W particles with little plastic deformation in the interior Al. Hydrocode simulations were conducted to gain an insight into this clustering behavior. Understanding of the mesoscale mechanisms may be useful to generate more efficient mesostructures and tailor the size of generated fragments based on the loading conditions. Funding was provided by ONR MURI N00014-07-1-0740 (Program Officer Dr. Clifford Bedford)

2:15PM D6.00003 Experimentally obtained hugoniot measurements for granular solids, DARCIE DENNIS-KOLLER, R. JASON SCHARFF, D. ANTHONY FREDENBURG, Los Alamos National Laboratory — Porous/granular materials are a class of materials where historical Hugoniot data is fraught with difficulty leading to unreliable data or extremely large associated errors. This presentation will present new experimental methods for obtaining reliable experimental Hugoniot data as well as attempt to describe the physical mechanisms responsible for anomalous behavior observed in distended systems.
2:30PM D6.00004 Explosive formation of coherent particle jets, DAVID FROST, JEAN-FREDERIC RUEL, ZOUYA ZAREI, SAM GOROSHIN, YANN GREGOIRE, McGill University, FAN ZHANG, DRDC Suffield, ALEC MILNE, AARON LONGBOTTOM, Fluid Gravity Engineering Ltd. — A high-speed jet of solid particles may be formed by detonating an explosive layer lining the outside of a conically-shaped volume of particles. Experiments have been carried out to determine the velocity history and the coherency of a particle jet formed using this shaped-charge arrangement. Important parameters include the cone angle, the ratio of the masses of the explosive and particles, and the particle size and density. Dense particles (e.g., iron) form thin, stable, coherent jets, whereas lighter particles (e.g., glass or Al) lead to more diffuse jets. The jet velocities observed experimentally were close to the predictions from a Gurney velocity formulation for conical geometry. The effects of cone angle and particle density on the jet formation and development were explored with calculations using a multimaterial hydrocode. The simulations indicate that the converging shock and Mach disk within the particle bed have a strong influence on the uniformity of the particle density field. With iron particles, the particle volume remains coherent whereas for glass particles, during the particle acceleration phase, the shock interactions within the particle bed cause the particles to be concentrated in a thin shell surrounding a low density region.

2:45PM D6.00005 Shock and Release of Duocel textregistered Aluminum Foam & Polyvinylidene Fluoride Composite Up to 20 GPa, WARREN MAINES, AFRL — Considerable interest in characterizing the dynamic response of heterogeneous materials under dynamic loading conditions exists because of their energy absorption and dissipation qualities. In the present study, 4 pores per centimeter 6101 T-6 aluminum foam, which was initially at 6-8% relative density of solid aluminum, was later compressed longitudinally to 20% relative density, (11 pores per centimeter) and filled with polyvinylidene fluoride (PVDF). The composite was then shocked up to 20 GPa using AFRL’s 60mn smooth bore powder gun. Results of these experiments will be compared to that of porous aluminum that was not filled. Further, computations at the meso-scale, which tracked well with experiments, highlighted the range of velocity distributions, as well as the damping caused by the addition of plastic. In particular, due to filler that was fairly close in density to the aluminum, the particle velocity variation was relatively low compared to porous foams from previous studies. The behavior of the composite was dominated by the presence of the plastic filled material, which demonstrated dissociation at pressures greater than 8 GPa.

Monday, July 8, 2013 1:45PM - 3:15PM – Session D7 CH.3 Chemistry: Energetic Material Initiation Grand Crescent - Christopher Berg, University of Illinois

1:45PM D7.00001 Simulations of the chemistry of shocked energetic materials on the nanosecond timescale, LAURENCE FRIED, Lawrence Livermore National Laboratory — The initiation of chemistry by a shock wave occurs through complex interactions between chemical and mechanical mechanisms. The first few nanoseconds after shock arrival is a crucial time period, where the initiation of exothermic chemical reactions leads to the growth of local hot spots. We are simulating these mechanisms in two ways. First, we are performing atomistic simulations of shocked TATB using a modified version of the ReaxFF force field. We have found that modification of ReaxFF is necessary in order to accurately model charge transfer and ionization under sustained high density conditions. We have simulated overdriven detonation waves in TATB using the multi-scale shock technique (MSST). In our simulations of overdriven shocked TATB, we find that large-scale graphitic structures encompassing thousands of atoms form after charge transfer and ionization under sustained high density conditions. We have simulated overdriven detonation waves in TATB using the multi-scale shock technique (MSST). In our simulations of overdriven shocked TATB, we find that large-scale graphitic structures encompassing thousands of atoms form after charge transfer and ionization under sustained high density conditions. We have successfully built a Femtosecond Stimulated Raman Spectroscopy (FSRS) system that works in tandem with our existing 400 nm broadband shaped pump (actinic pump) and 400-700 nm Transient Absorption (TA) probe experiment. This gives us a unique capability to characterize the complex photo-chemical reactions that occur when time dependent electric fields interact with energetic materials. Steering the outcome of a chemical reaction with light requires optimally shaped ultrashort laser pulses to guide energy flow along desired reaction coordinate pathways. The ability to measure the complex photo-chemical dynamic molecular vibrations is key to not only understanding but controlling the photodecomposition mechanisms of energetic materials. We have successfully built a Femtosecond Stimulated Raman Spectroscopy (FSRS) system that works in tandem with our existing 400 nm broadband shaped pump (actinic pump) and 400-700 nm Transient Absorption (TA) probe experiment. This gives us a unique capability of photo-exciting energetic materials with an actinic shaped broadband femtosecond pump pulse and measuring the resulting dynamics simultaneously using FSRS and TA. The measured evolution of the TA and, more importantly, the vibrational spectrum during the photodecomposition transformation provides key structural data on the reaction mechanisms. We have tested our new capability on both energetic and non-energetic materials and have observed vibrational dynamic changes suggesting possible decomposition mechanisms.

2:15PM D7.00002 Toward quantum controlled initiation of energetic materials, MARGO GREENFIELD, SHAWN MCGRANE, JASON SCHARRFF, KATHRYN BROWN, DAVID MOORE, Los Alamos National Laboratory, HERCULES TEAM — Successful quantum controlled initiation requires understanding the photochemical reactions that occur when time dependent electric fields interact with energetic materials. Steering the outcome of a chemical reaction with light requires optimally shaped ultrashort laser pulses to guide energy flow along desired reaction coordinate pathways. The ability to measure the complex photo-chemical dynamic molecular vibrations is key to not only understanding but controlling the photodecomposition mechanisms of energetic materials. We have successfully built a Femtosecond Stimulated Raman Spectroscopy (FSRS) system that works in tandem with our existing 400 nm broadband shaped pump (actinic pump) and 400-700 nm Transient Absorption (TA) probe experiment. This gives us a unique capability of photo-exciting energetic materials with an actinic shaped broadband femtosecond pump pulse and measuring the resulting dynamics simultaneously using FSRS and TA. The measured evolution of the TA and, more importantly, the vibrational spectrum during the photodecomposition transformation provides key structural data on the reaction mechanisms. We have tested our new capability on both energetic and non-energetic materials and have observed vibrational dynamic changes suggesting possible decomposition mechanisms.

2:30PM D7.00003 Study of the laser-induced decomposition of energetic materials at static high-pressure by time-resolved absorption spectroscopy, PHILIPPE HEBERT, CHARLES SAINT-AMANS, CEA DAM Le Ripault, BP16, 37260 MONTS, France — A detailed description of the reaction rates and mechanisms occurring in shock-induced decomposition of condensed explosives is very important to improve the predictive capabilities of shock-to-detonation transition models. However, direct measurements of such experimental data are difficult to perform during detonation experiments. By coupling pulsed laser ignition of an explosive in a diamond anvil cell (DAC) with time-resolved streak camera recording of transmitted light, it is possible to make direct observations of deflagration phenomena at detonation pressure. We have developed an experimental set-up that allows combustion front propagation rates and time-resolved absorption spectroscopy measurements. The decomposition reactions are initiated using a nanosecond YAG laser and their kinetics is followed by time-resolved absorption spectroscopy. The results obtained for two explosives, nitromethane (NM) and HMX are presented in this paper. For NM, a change in reactivity is clearly seen around 25 GPa. Below this pressure, the reaction products are essentially carbon residues whereas at higher pressure, a transient absorption feature is first observed and is followed by the formation of a white amorphous product. For HMX, the evolution of the absorption as a function of time indicates a multi-step reaction mechanism which is found to depend on both the initial pressure and the laser fluence.
2:45PM D7.00004 Ultrafast laser diagnostics for studies of shock initiation in energetic materials, DARCY FARROW, BROOK JILEK, URAYAMA JUNJI, JAN KHOL, SEAN KEARNEY, Sandia National Laboratories — Ultrafast laser diagnostics have opened new pathways for investigation of shock physics and initiation of energetic materials. Recent work (Belome LANL/Armstrong LLNL) has demonstrated that short laser pulses can be utilized for direct laser drive and coupled with imaging, spectroscopic, and interferometric tools for studies of dynamic shock loading on picosecond time scales. At Sandia, we are developing diagnostic platforms which extend this earlier work including: (1) Ultrafast Shock Interferometry (USI) (Armstrong LLNL) for tabletop measurement of Hugoniot/Equation-of-state data and characterization of shock structure in heterogeneous materials with micron spatial resolution; (2) coherent Raman diagnostics, including Coherent anti-Stokes Raman spectroscopy (CARS) and stimulated Raman scattering (SRS) for measurement of temperature and dynamic changes in chemical bonding; and (3) femtosecond transient absorption spectroscopy, which can monitor shock-induced shifts in electronic structure, which have been proposed to drive rapid chemical changes behind the shock front. We are pursuing a path where each of these tools is being developed independently and then combined for the study of shock physics studies in thin films of energetic materials. At the APS/SCCM, we will describe the details of our measurement systems, as well as recent progress toward new laser-diagnostic data on inert/explosive thin-film samples.

3:00PM D7.00005 Toward a Role of Light Absorption in Initiation Chemistry of Shocked HMX single Crystals and Crystalline High Explosives1, IGOR PLAKSIN, L. RODRIGUES, ADAI, Un of Coimbra — Question which mechanism is driving radiation-induced reactions, thermal or athermal becomes a subject of conflicting discussions. Major challenge of this work is to identify at micro- (sub-granular), meso- (grain level) and macro-scale roles of these two mechanisms in triggering initiation chemistry in HMX-based HEs. Four acceptor-patterns were tested at 20 GPa input pressure: single HMX crystal-in-water, HMX/water-slurry, PBX(HMX/HTPB) & inert PBX-simulant (HMX-particles replaced by crystalline sucrose). Scenario of reaction onset-localizations-dissipation was spatially resolved using Multi-Channel Optical Analyzer MCOA-USI (96 channels, 100um-spatial accuracy, 0.2ns-timesresolution, 450-850 nm-spectral range) through real-time panoramic recording emitted reaction light and shock field in standard optic monitor. Experiments reveal a dual nature of initiation chemistry: athermal and thermal. Single-crystal tests disclose origination of photo-induced reactions downstream of emitting reaction spot due to intensified radiation absorption in surface micro-defects. Polycrystalline samples reveal cyclic reproducibility of radiation-induced thermal precursors in which radiation absorption causes thermal expansion/phase-changes of HMX-grains resulting in oscillating detonation.

Monday, July 8, 2013 3:30PM - 5:15PM –
Session E1 ME.4 Strength IV Grand Ballroom I - Tracy Vogler, Sandia National Laboratories

3:30PM E1.00001 Using Growth and Arrest of Richtmyer-Meshkov Instabilities and Lagrangian Simulations to Study High-Rate Material Strength, MICHAEL PRIME, DIANE VAUGHAN, DEAN PRESTON, DAVID ORO, WILLIAM BUTTLER, Los Alamos National Laboratory — Rayleigh-Taylor instabilities have been widely used to study the deviatoric (flow) strength of solids at high strain rates. More recently, experiments applying a supported shock through mating surfaces (Atwood number = 1) with geometrical perturbations have been proposed for studying strength at strain rates up to 107/sec using Richtmyer-Meshkov (RM) instabilities. Buttler et al. [J. Fluid Mech., 2012] recently reported experimental results for RM instability growth but with an unsupported shock applied by high explosives and the geometrical perturbations on the opposite free surface (Atwood number = -1). This novel configuration allowed detailed experimental observation of the instability growth and arrest. We present results and detailed interpretation from numerical simulations of the Buttler experiments on copper. Highly-resolved, two-dimensional simulations were performed using a Lagrangian hydrocode and the Preston-Tonks-Wallace (PTW) strength model. The model predictions show good agreement with the data in spite of the PTW model being calibrated on lower strain rate data. The numerical simulations are used to 1) examine various assumptions previously made in an analytical model, 2) to estimate the sensitivity of such experiments to material strength and 3) to explore the possibility of extracting meaningful strength information in the face of complicated spatial and temporal variations of stress, pressure, and temperature during the experiments.

3:45PM E1.00002 Inferring yield strength in α-phase cerium from a Richtmyer-Meshkov Instability1, FRANK CHERNE, BRIAN JENSEN, KYLE RAMOS, JOHN YEAGER, GUY DIMONTE, GUILLERMO TERRONES, MICHAEL PRIME, Los Alamos National Laboratory, KAMEL FEZZAA, APS, Argonne National Laboratory, CHARLES OWENS, Los Alamos National Laboratory — Recent experiments on the 12-mm gas gun known as IMPULSE at the Advanced Photon Source (Argonne, IL) were performed to examine Richtmyer-Meshkov instability (RMI) growth for cerium samples shocked into the α-phase. The high resolution images that have been obtained using X-ray phase contrast imaging show spike growth from a machined RMI surface with unprecedented spatial resolution (2-3 microns). Applying the theory developed by G. Dimonte, et al. [PRL 107 265402 (2011)], we have inferred the yield stress for cerium which was shocked into the α-phase. We observed that the yield stress decreased as the melt boundary was approached similar to copper. Because the experiments were not performed using an ideal sinusoidal perturbation, molecular dynamics simulations and continuum calculations have been performed looking at the effect of the surface shape used in this work. In this work, a detailed discussion of the analysis will be presented along with a comparison of our calculations with available experimental data.

4:00PM E1.00003 Investigating iron material strength during phase transitions using Rayleigh-Taylor growth measurements1, CHANNING HUNTINGTON, JON BELOF, KERRI BLOBLAUM, ROB CAVALLO, NATALIE KOSTINSKI, BRIAN MADDIX, MARK MAY, HYE-SOOK PARK, CHRISTOPHER PLECHATY, SHON PRISBREY, BRUCE REMINGTON, ROBERT RUDD, DAVID SWIFT, RUSSELL WALLACE, MICHAEL WILSON, Lawrence Livermore National Laboratory — A solid-solid phase transition between the bcc (α) and hcp (ε) lattice structures in iron is known to occur as the material is compressed. When kept below its melting point, an effective increase in the macroscopic strength of the material accompanies this phase transition. Understanding the strength of iron throughout the deformation process is important for improving models of planetary structure, including interpretation of seismic measurements on Earth. To explore iron strength at high pressures and strain rates, we have performed experiments at the OMEGA laser. The laser drive produces a pressure near 1 Mbar on a thin Fe disk with a sinusoidal ripple pattern imposed on its face. The ripples seed the Rayleigh-Taylor (RT) instability, the growth of which is suppressed by the material strength of the sample. The ripple amplitude is diagnosed with x-ray radiography, and their growth is compared to values from simulations using different material strength models. This work will be compared to previous, similar experiments at 0.1 – 0.3 Mbar pressures (J. Beol et al., AIP Conf. Proc. 2012).

1 This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
4:15PM E1.00004 Solid state Rayleigh-Taylor measurements in Ta and V at high pressures and strain rates\(^1\), BRUCE A. REMINGTON, HYE-SOOK PARK, ROBERT CAVALLO, SHON PRISBREY, ROBERT RUDD, CHRIS PLECHATY, CHRIS WEHRENBERG, BRIAN MADDOX, NATALIE KOSTINSKI, MATTHEW TERRY, C.M. HUNTINGTON, LLNL — We will report on Rayleigh-Taylor (RT) strength experiments in solid-state driven foils of vanadium and tantalum at high strain rates (~1.67 1/s) and high pressures (~1 Mbar), where softening (a decrease in strength) is observed when the strains get large. When the single-mode RT bubble penetration in this plastic flow regime reaches ~20-30% of the initial foil thickness, the inferred high strength in the foils starts to drop. In the extreme, this drop in strength may be an indication of incipient failure. We will discuss the similarities and differences between the observed softening in the V-RT and Ta-RT experiments, and consider the implications for future planned experiments on the National Ignition Facility (NIF) at higher pressures (~5 Mbar), but similar strain rates.

\(^1\)Prepared by LLNL under Contract DE-AC52-07NA27344

4:30PM E1.00005 Hydrodynamic instabilities and dynamic strength. RAEVSKY VICKTOR, None — The paper presents results of numerical-theoretical and experimental investigations of influence of shear strength on growth of the Richtmyer-Meshkov instability and the Rayleigh-Taylor instability. It is revealed that, for monochromatic perturbations at accelerated boundary of a solid, there are the critical conditions when the perturbation growth is limited. High sensitivity of perturbation growth to dynamic strength near the stability boundary allowed to develop the method for determination of dynamic strengths of substances in wide range of pressures and strain rates (? ~ 10 ÷ 300 GPa, strain rate ~ 10E4 ÷ 10E7 1/s). The paper includes setup and results of series of tests devoted to investigation of dynamic strengths of some metals (?t, ?u, AL, Be).

4:45PM E1.00006 Dynamic strength and instabilities of Rayleigh-Taylor and Richtmayer-Meshkov, VICTOR RAEVSKY, VNIEFF — Will require a translator

Monday, July 8, 2013 3:30PM - 5:30PM –
Session E2 CM.2 Phase Transitions: Melting –
Grand Ballroom II - Nenad Velisavljevic, Los Alamos National Laboratory

3:30PM E2.00001 Melting curve of metals evidenced by X-ray diffraction. AGNES DEWA ELE, CEA — There has been a consistent pattern of disagreement between the determinations of high pressure melting by two experimental techniques, the static laser-heated diamond anvil cell (LH DAC) and the dynamic shock wave compression. For several elements, “high” and “low” melting points have been measured by shock compression and LHDAC, respectively. The difference could exceed one thousand of K. We have revisited the melting curve of a few metals in a LHDAC: lead, tantalum, beryllium and iron. We have used an alternative diagnostic of melting, based on X-ray diffraction instead of optical detection. The melting curves obtained with this diagnostic are in correct agreement with shock wave data. Movements of the sample surface, which were previously interpreted as a melting signature, could be due to a fast recrystallization of the solid sample. This fast recrystallization is evidenced by X-ray diffraction up to several hundreds of degrees below melting for some metals.

4:00PM E2.00002 Guest Chain “Melting” in Incommensurate Host-Guest Potassium. EMMA MCBRIDE, KEITH MUNRO, MALCOLM MCMAHON, SUPA, School of Physics and Astronomy, and Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh, UK — Upon increasing pressure the group-I elements transform from close-packed structures (bcc and fcc) to a series of low-symmetry complex structures. Residing in the middle of the group, potassium (K) has numerous structures in common with its neighbours, and, in fact, is remarkably structurally similar to sodium (Na) and rubidium (Rb). For example, the post-fcc transition in K is to a composite incommensurate host-guest structure (t19f), and the host structure of this phase is isostructural with that found in Na and Rb. Previously we have reported that below ~16.7 GPa, the Bragg peaks from the guest component of t19f-Rb broaden considerably, signalling a loss of the inter-chain correlation, or a “melting” of the chains. Furthermore, in t19f-Na above 125 GPa, the Bragg peaks from the guest component are also broadened, suggesting that the guest chains are also nearly “melted.” During studies of the melting curve of K, we observed that the guest peaks from t19f-K broaden dramatically on heating. Here we report single-crystal, quasi-single-crystal, and powder synchrotron x-ray diffraction measurements of t19f-K to 50 GPa and 800 K, which allowed a detailed study of this chain “melting” transition. The order-disorder transition is clearly visible over a 30 GPa pressure range, and there are significant changes in the gradient of the phase boundary, which may be influenced by the nature of the guest structure. Furthermore, data extending the melting curve will also be presented.

4:15PM E2.00003 Melting of lithium at high pressure, SHANTI DEEMYAD, ANNE MARIE SCHAFFER, University of Utah — At ambient pressure, lithium is the lightest metallic element and the prototype of a simple metal, with a nearly spherical Fermi surface. The structural and electronic properties of lithium at high densities are highly counterintuitive. Under high pressure, lithium undergoes a series of symmetry breaking structural phase transitions and a theoretically predicted complex melting curve. In addition, because of its low atomic mass, lithium may behave as a quantum solid. If this is the case, its melting transition would resemble that of metallic hydrogen, and is of critical interest. Direct observation of the melting transition of lithium under high pressure has been challenging due to its strong reactivity. In this talk I will review the unusual physics of lithium at extreme pressures and present our recent experimental result on high pressure melting curve of lithium.

4:30PM E2.00004 High pressure melting of lithium, ANNE MARIE SCHAFFER, WILLIAM TALMADGE, SCOTT TEMPLE, SHANTI DEEMYAD, University of Utah — The electrical resistivity of metals exhibit a well documented sharp increase near the melting temperature. The electrical resistivity of lithium was measured using a quasi-four point probe inside a diamond anvil cell. The sharp increase in the resistivity upon melting, complemented by visual observations, was used to measure the melting curve of lithium from ambient pressure to 64 GPa. Using the same experimental configuration, the electrical resistivity measurements of lithium have been expanded.

4:45PM E2.00005 Dynamic Melting of Highly Compressed Nitrogen\(^1\), DANE TOMASINO, CHOONG-SHIK YOO, Department of Chemistry, Institute of Shock Physics, Washington State University, Pullman, Washington 99164 — Nitrogen exhibits a fascinating high-pressure polymorphism in solid along with the predicted transition to a conducting polymer in liquid. The solid-liquid phase boundary, however, is still the subject of debate – not well understood. This is, in part, due to a lacking of proper in-situ structural/chemical diagnostic technique capable of probing hot dense nitrogen phases at high pressures and temperatures. The challenge is mainly due to high mass and thermal diffusivity and chemical reactivity of hot dense fluids. To remedy this situation, we have applied the time-resolved Raman spectroscopy on laser-heated nitrogen in diamond anvil cells. In this experiment, the onset of melting was determined in-situ by probing the discontinuous spectral change in nitrogen vibrors during rapid isochoric heating, while the temperature was measured through time-resolved thermal spectro-radiometry.

\(^1\)The present study has been supported by NSF-DMR (Grant No. 1203834) and DTRA (HDTRA1-12-01-0020).
5:00PM E2.00006 Atomistic modeling of graphite melting, NIKITA OREKHOV, VLADIMIR STEGAIOLOV, JIHT RAS — Graphite melting properties have been the subjects of debate for many years due to discrepancy in experimental data. We report here molecular dynamic simulations of graphite melting with the semiempirical bond-order potential AIREBO. As a result in the pressure range up to 14 GPa the graphite melting line was obtained and properties of liquid carbon were investigated. For the superheated graphite the melting front velocity dependencies on temperature were calculated to verify the values of melting temperatures.

5:15PM E2.00007 Melting of GaN — still open problem, S. POROWSKI, B. SADOVYI, S. GIERLOTKA, A. PRESZ, I. GRZEZORY, Institute of High Pressure Physics PAS, Sokolowska str., 29/37, 01-142 Warsaw, Poland, I. PETRUSHA, V. TURKEVICH, D. STATIICHUK, Dep. of Synthesis and Sintering of Superhard Materials, V. N. Bakul Institute for Superhard Materials NAS Ukraine, Avtozavodska str., 2, Kyiv, 04074, INSTITUTE OF HIGH PRESSURE PHYSICS PAS, SOKOLOWSKA STR., 29/37, 01-142 WARSAW, POLAND TEAM, V. N. BAKUL INSTITUTE FOR SUPERHARD MATERIALS NAS UKRAINE, AVTOZAVODSKA STR., 2, KYIV, 04074, UKRAIN TEAM — In this work, thermal stability of GaN single crystals at pressure up to 9.0 GPa and temperature up to 3400 K has been studied. According to [1] the congruent melting of GaN occurs at 2533 K at pressure above 6.0 GPa. Results obtained in our study are not in agreement with this observation. In whole pressure and temperature range we observed that GaN decomposes to N2 gas and liquid gallium solution of nitrogen. The p-T decomposition curve which has been established is consistent with previously reported data for lower pressures and temperatures [2]. Also corresponding solubility of nitrogen in the liquid gallium has been evaluated by measuring the weight of crystals grown from solution at cooling of the system. At the highest pressure 17 at. % solubility was observed which is still significantly lower than 50 at. % required for stoichiometric melt.


Monday, July 8, 2013 3:30PM - 5:30PM —
Session E3 NT.2 Novel Techniques: PCI/2D Visar Fifth Avenue - Stefan Turneaure, Washington State University

3:00PM E3.00001 Compression and Shear of Tantalum to 64 GPa, YANZHANG MA, Department of Mechanical Engineering, Texas Tech University, Lubbock TX 79409, USA, WENGÉ YANG, CHENG JI1, High Pressure Synergetic Consortium, Carnegie Institution of Washington, Argonne, IL 60439, USA, YANG GAO, Department of Mechanical Engineering, Texas Tech University, Lubbock TX 79409, USA, OLIVER TSCHAUNER, High Pressure Science and Engineering Center, University of Nevada, Las Vegas, NV 89154, USA, STANISLAV SINOEIKIN, High Pressure Collaborative Access Team, Geophysical Laboratory, Carnegie Institution of Washington, Argonne, IL 60439, USA — It has been reported that the β-phase (body-centered-cubic) of tantalum (Ta) is stable to pressures over mega-bar under hydrostatic compression. [1] However, the shock compression clearly indicates its transformation to the ω-phase (hexagonal) at 45 GPa. [2] Theoretical work suggests that the shear might have played an important role in inducing this phase transformation. [3] Here we report our experimental results on the effects of pressure and shear by use of a rotational diamond anvil cell and the synchrotron X-ray diffraction. The results indicate that under extensive shear and pressures over 60 GPa, Ta remains stable in the β phase.


1 Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA

3:45PM E3.00002 Laser Interferometry Measurements in Starphire® Soda-Lime Glass Shocked to 14 GPa, AARON GUNDERSON, YOSHIMASA TOYODA, YOGENDRA GUPTA, Washington State University — Symmetric plate impact experiments were conducted on Starphire® samples at peak stresses varying between 4-14 GPa, and laser interferometry was used to monitor the particle velocity histories at the sample-impactor interface. A few hundred ns after impact, the lowest stress experiments exhibited either decreasing particle velocity or fluctuations in particle velocity. The higher stress experiments did not show these features and exhibited a constant particle velocity throughout. Sample compression causes a change in the optical path length, resulting in the observed particle velocity to be offset from the actual particle velocity at the sample-impactor interface. The actual particle velocities were known independently from the projectile velocity measurements, due to the symmetric nature of the impact in the present work. Observed and actual particle velocities were compared to obtain velocity corrections for the range of compressions examined. The present results were compared to published velocity correction data for Starphire®. While the present data agree with the published data at the lowest stresses, the two sets of results do not agree at higher stresses. Potential reasons for this disagreement are presented. Work supported by the DOE/NNSA.

4:00PM E3.00003 Shock wave viscosity measurements, PETER CELLIERIS, Lawrence Livermore National Laboratory — Several decades ago a method was proposed and demonstrated to measure the viscosity of fluids at high pressure by observing the oscillatory damping of sinusoidal perturbations on a shock front [1]. A detailed mathematical analysis of the technique carried out subsequently by Miller and Ahrens [2] revealed its potential, as well as a deep level of complexity in the analysis. We revisit the ideas behind this technique in the context of a recent experimental development: two-dimensional imaging velocimetry. The new technique allows one to capture a broad spectrum of perturbations down to few micron scale-lengths imposed on a shock front from an initial perturbation. The detailed evolution of the perturbation spectrum is sensitive to the viscosity in the fluid behind the shock front. Initial experiments are aimed at examining the viscosity of shock compressed SiO2 just above the shock melting transition.


1 This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

4:30PM E3.00004 Dynamic Loading to Study Damage Evolution in Heterogeneous Microstructures using IMPULSE at the Advanced Photon Source. JOHN YEAGER, KYLE RAMOS, BRIAN JENSEN, DARLA GRAFF THOMPSON, Los Alamos National Laboratory, ADAM IVerson, CARL CARLSON, National Security Technologies, LLC, KAMEL FEZZAA, Argonne National Laboratory, DAN HOOKS, Los Alamos National Laboratory — The performance, safety, and thermo-mechanical response of heterogeneous materials such as plastic-bonded explosives (PBXs) is inherently linked to microstructural phenomena. Experimental resolution of the physics and chemistry of the microstructure at appropriate length scales, both at ambient conditions and under dynamic loading, are highly desirable to develop new materials and models to predict their behavior. Here, the dynamic response of several heterogeneous materials is studied with real-time, in situ, spatially resolved measurements using the IMPULSE platform at the Advanced Photon Source (APS) at Argonne National Laboratory. Known PBX damage mechanisms such as void collapse, crack propagation, and plasticity or material flow are imaged at ultrafast speeds under shock loading conditions with simultaneous X-ray phase contrast imaging (PCI). PCI at APS beam line 32-ID is an improvement over conventional techniques because it detects phase shifts in the transmitted X-ray beam, making PCI an ideal technique to image interfaces (i.e. heterogeneity) with high spatial resolution (2μm) in-plane. IMPULSE experiments are compared with similar experiments at other length and time scales to discern relevant processing-structure-properties relationships for several PBX materials.

4:45PM E3.00005 Numerical re-focusing of 2d-VISAR data¹. DAVID ERSKINE, RAYMOND SMITH, Lawrence Livermore National Laboratory, CYNTHIA BOLME, Los Alamos National Laboratory, SUZANNE ALI, PETER CELLIERS, GILBERT COLLINS, Lawrence Livermore National Laboratory — Two dimensional velocity interferometer (2d-VISAR) data can be treated as a kind of hologram, since fringes recorded by the interferometer manifest both phase and magnitude information about changes in the optical field of the target, over an image. By the laws of diffraction, knowledge of the optical field at one focal plane can be used to calculate the optical field at another focal plane. Hence a numerical re-focusing operation can be performed on the data post-experiment, which can bring into focus narrow features that were recorded in an out of focus configuration. Demonstration on shocked Si data and theoretical models are shown.

5:00PM E3.00006 Imaging the propagation of shock waves with both high temporal and high spatial resolution using XFELs, ANDREAS SCHROPP, SLAC National Accelerator Laboratory, 2575 Sand Hill Rd., Menlo Park, CA 94025, USA — The emergence of x-ray sources of the fourth generation, so called x-ray free-electron lasers (XFELs), comes along with completely new research opportunities in various scientific fields. During the last year we developed an x-ray microscope based on beryllium compound refractive lenses (Be-CRLs), which is especially optimized for the XFEL environment and provides focusing capabilities down to 100nm and even below. Based on magnified x-ray phase contrast imaging, this new setup enables us to pursue high-resolution x-ray imaging experiments with single XFEL-pulses. In a first experiment, carried out at the Matter in Extreme Conditions (MEC) endstation of the LCLS, the performance of the instrument was investigated by direct imaging of shock waves in different materials. The shock wave was induced by an intense 150ps optical laser pulse. The evolution of the shock wave was then monitored with the XFEL-beam. In this contribution we report on first analysis results of phase contrast imaging of shock waves in matter.

In collaboration with Brice Arnold, Eric Galtier, Hae Ja Lee, Bob Nagler, Jerome Hastings, SLAC National Accelerator Laboratory, 2575 Sand Hill Rd., Menlo Park, CA 94025, USA; Damian Hicks, Yuan Ping, Gilbert Collins, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, USA; and Robert Hoppe, Vivienne Meier, Jens Patomml, Frank Seiboth, Christian Schröer, Institute of Structural Physics, Technische Universität Dresden, D-01062 Dresden, Germany.

Monday, July 8, 2013 3:30PM - 5:30PM – Session E4 MB Blast Injury Vashon - James Leighs, Cranfield University

3:30PM E4.00001 Integrated Experimental Platforms to Study Blast Injuries: a Bottom-Up Approach¹. CHIARA BO, Institute of Shock Physics, Imperial College London — Developing a cellular and molecular understanding of the nature of traumatic and post-traumatic effects of blast events on live biological samples is critical for improving clinical outcomes. To investigate the consequences of pressure waves upon cellular structures and the underlying physiological and biochemical changes, we are using an integrated approach to study the material and biological properties of cells, tissues and organs when subjected to extreme conditions. In particular we have developed a confined Split Hopkinson Pressure Bar (SHPB) system, which allows us to subject cells in suspension or in a monolayer to compression waves of the order of few MPa and duration of hundreds of microseconds. The chamber design also enables recovery of the biological samples for cellular and molecular analysis. Specifically, cell survivability, viability, proliferation and morphological changes are investigated post compression for different cell populations. The SHPB platform, coupled with Quasi-Static experiments, is also used to determine stress-strain curves of soft biological tissues under compression at low, medium and high strain rates. Samples are also examined using histological techniques to study macro- and microscopical changes induced by compression waves. Finally, a shock tube has been developed to replicate primary blast damage on organs (i.e. mice lungs) and cell monolayers by generating single or multiple air blast of the order of kPa and few milliseconds duration. This platform allows us to visualize post-traumatic morphological changes at the cellular level as a function of the stimulus pressure and duration as well as biomarker signatures of blast injuries. Adapting and integrating a variety of approaches with different experimental platforms allows us to sample a vast pressure-time space in terms of biological and structural damage that mimic blast injuries and also to determine which physical parameters (peak pressure, impulse) are contributing to the injury process. Moreover, understanding biological damage following blast events is crucial to developing novel clinical approaches to detect and treat traumatic injury pathologies.

¹Prepared by LLNL under Contract DE-AC52-07NA27344.

4:00PM E4.00002 Microjet Penetrator - medical use of laser induced shock waves and bubbles

JACK J. YOH, Seoul National University — The laser-driven microjet penetrator system accelerates liquids drug and delivers them without a needle, which is shown to overcome the weaknesses of existing piston-driven jet injectors. The system consists of two back-to-back chambers separated by a rubber membrane, one containing “driving” water behind another of the liquid drug to be delivered. The laser pulse is sent once, and a bubble forms in the water chamber, which puts elastic strain on the membrane, causing the drug to be forcefully ejected from a miniature nozzle in a narrow jet of 150 micron in diameter. The impacting jet pressure is higher than the skin tensile strength and thus causes the jet to penetrate into the targeted depth underneath the skin. Multiple pulses of the lasers increase the desired dosage. The experiments are performed with commercially available Nd:YAG and Er:YAG lasers for clinical applications in laser dermatology and dentistry. The difference in bubble behavior within the water chamber comes from pulse duration and wavelength. For Nd:YAG laser, the pulse duration is very short relative to the bubble lifetime making the bubble behavior close to that of a cavitation bubble (inertial), while in Er:YAG case the high absorption in water and the longer pulse duration change the initial behavior of the bubble making it close to a vapor bubble (thermal). The contraction and subsequent rebound for both cases were seen typical of cavitation bubble. The laser-induced microjet penetrators generate velocities which are sufficient for delivery of drug into a guinea-pig skin for both laser beams of different pulse duration and wavelength. We estimate the typical velocity within 30-80 m/s range and the breakup length to be larger than 1 mm, thus making it a contamination-free medical procedure. Hydrodynamic theory confirms the nozzle exit jet velocity obtained by the microjet system. A significant increase in the delivered dose of drugs is achieved with multiple pulses of a 2.9µm Er:YAG laser at 250µs pulse duration. At this wavelength, the beam is best absorbable by water. Further, to increase the bubble size, a sapphire based fiber tip is entered into a water chamber as a beam is gathered at the bottom of this fiber tip’s conical end, which is polished at an angle graduated from 30° over the full core diameter. The power density at the exit of the conical fiber tip is increased in comparison with the direct radiation at water. The water superheats and thus a larger bubble forms right at the tip. The bubble is typically an elongated (stretched) shape in case of a direct laser irradiation in water, but when light is irradiated through a conical fiber tip, the resulting bubble is an enlarged spherical bubble which is several times larger in its volume when compared to the direct beam radiation in water. In this talk, a review of our recent research effort in achieving high-throughput injection of drug via the microjet penetrator is given with its potential medical applications.

3The financial support is provided by National Research Foundation of Korea (DOYAK-2010).

4:30PM E4.00003 Traumatic eye injuries as a result of blunt impact

CHIARA CLEMENTE, University of Cassino and Southern Lazio, LUCA ESPOSITO, PALMER - Scientific and Technology Park of Southern Lazio, NICOLA BONORA, University of Cassino and Southern Lazio, JEROME LIMIDO, JEAN-LUC LACOME, IMPETUS-AFEA, TOMMASO ROSSI, Ophthalmic Hospital of Rome — The detachment or tearing of the retina in the human eye as a result of a collision is a phenomenon that occurs very often. This research is aimed at identifying and understanding the actual dynamic physical mechanisms responsible for traumatic eye injuries accompanying blunt impact, with particular attention to the damage processes that take place at the retina. To this purpose, a numerical and experimental investigation of the dynamic response of the eye during an impact event was performed. Numerical simulation of both tests was performed with IMPETUS-FAE, a general non-linear finite element software which offers NURBS finite element technology for the simulation of large deformation and fracture in materials. Computational results were compared with the experimental results on fresh enucleated porcine eyes impacted with airsoft pellets. The eyes were placed in a container filled with 10 percent ballistic gelatin simulating the fatty tissue surrounding the eye. A miniature pressure transducer was inserted into the eye bulb through the optic nerve in order to measure the pressure of the eye during blunt-projectile impacts. Each test was recorded using a high speed video camera. The ocular injuries observed in the impacted eyes were assessed by an ophthalmologist in order to evaluate the correlation between the pressure measures and the risk of retinal damage.

4:45PM E4.00004 Prediction of Shock-Induced Cavitation in Water

AARON BRUNDAGE, Sandia National Laboratories — Fluid-structure interaction problems that require estimating the response of thin structures within fluids to shock loading has wide applicability. For example, these problems may include underwater explosions and the dynamic response of ships and submarines; and biological applications such as Traumatic Brain Injury (TBI) and wound ballistics. In all of these applications the process of cavitation, where small cavities with dissolved gases or vapor are formed as the local pressure drops below the vapor pressure due to shock hydrodynamics, can cause significant damage to the surrounding thin structures or membranes if these bubbles collapse, generating additional shock loading. Hence, a two-phase equation of state (EOS) with three distinct regions of compression, expansion, and tension was developed to model shock-induced cavitation. This EOS was evaluated by comparing data from pressure and temperature shock Hugoniot measurements for water up to 400 kbar, and data from ultrasonic pressure measurements in tension to ~0.3 kbar, to simulated responses from CTH, an Eulerian, finite volume shock code. The new EOS model showed significant improvement over pre-existing CTH models such as the SESAME EOS for capturing cavitation.

5:00PM E4.00005 On the interaction between blast wave and reticulated foams

JAMES WILGEROTH, WILLIAM PROUD, THUY-TIEN NGOC NGUYEN, Imperial College London, INSTITUTE OF SHOCK PHYSICS TEAM, CENTRE FOR BLAST INJURY STUDIES TEAM — Injuries to the tympanic membrane (ear drum) and inner ear are particularly common in individuals subjected to blast overpressure, such as military personnel engaged in conflict. Consequently, there is a demand for improved auditory protection systems, which are capable of both preventing this type of injury while providing maximum situational awareness to the user. In this study, a number of reticulated (open cell) foams have been subjected to dynamic compression using shock tube apparatus. Specific effects of porosity; relative density, which is determined by the ratio of cellular material to solid material from which the foam is made; sample thickness; incident pressure; and shock pulses of varying timescale upon the evolution of peak overpressure behind foam samples have been investigated. In addition, the use of Schlieren imaging techniques has allowed for detailed examination of gaseous flow at the rear surface of shocked foam samples.

5:15PM E4.00006 Shockless compression (loading rate of 5 x 10^12/s) of ballistic gel to 1 GPa

YOSHIMASA TOYODA, YOGENDRA GUPTA, Washington State University — Ballistic gel has been commonly used as a soft tissue simulant in ballistic experiments for decades. However, experimental results needed to develop material models at stresses and loading rates comparable to ballistic loading are lacking. To examine the dynamic response of ballistic gel at the desired stresses and loading-rates, shockless uniaxial-strain compression experiments were conducted on 10 and 20 weight percent ballistic gel to 1 GPa peak stress. Plate-impact experiments were conducted using the following target configurations: fused silica/gel/PMMMA optical window. The anomalous compression of fused silica resulted in a near-linear, shockless compression (5 x 10^12/s). Velocity histories at the front and the rear ballistic gel interfaces were simultaneously recorded using laser interferometry (VISAR). From the velocity histories, the loading paths (in the pressure-volume plane) for each gel concentration were determined. The 20 wt.% ballistic gel resulted in the steeper loading path, demonstrating that the dynamic compression response of 20 wt.% gel is stiffer than the 10 wt.% gel. The wave profiles and the quantitative results will be discussed. Dr. D. P. Dandekar (ARL) is thanked for his help and insightful discussions. Work supported by ARL and DOE/NNSA.

Monday, July 8, 2013 3:30PM - 5:30PM – Session E5 LS Large Scale Experiments I

Cascade I - Brad Wallin, Lawrence Livermore National Laboratory
3:30PM E5.00001 Capabilities of the Extreme Conditions Beamline at PETRA III, DESY  
HANNS-PETER LIERMANN, ZUZANA KONOPKOVÁ, Photon Sciences, Deutsches Elektronen Synchrotron, WOLFGANG MORGENRoth, Department of Crystallography, University of Frankfurt, ANDRE ROTHKIRCH, EUGEN WITTICH, JAN-TORBEN DELITZ, ANITA EHNES, Photon Sciences, Deutsches Elektronen Synchrotron — At the end of 2010 the Extreme Conditions Beamline (ECB) at PETRA III received first beam and entered the commissioning phase. Since 2012 we are offering beamtime to general users to conduct a variety of different experiments such as powder and single diffraction in the laser/resistive heated and cryogenically cooled Diamond Anvil Cell (DAC). Particularly attractive has been our ability to conduct diffraction experiments at high energies of 60 and 77 keV for pair distribution function (PDF) studies as well as possibility to preform time resolved powder diffraction experiments at 26 and 43 keV with a maximum time resolution of 15 Hz. Within we present some of the current capabilities of the beamline as well as future plans to promote single crystal diffraction at high pressures and temperatures using both monochromatic and pink beam. Finally, we emphasis the present and future time resolved capabilities to conduct powder and single crystal diffraction experiments under dynamic compression and heating conditions in the DAC.

3:45PM E5.00002 X-ray Diffraction and Multi-Frame Phase Contrast Imaging Diagnostics for IMPULSE at the Advanced Photon Source  
ADAM IVERSON, CARL CARLSON, National Security Technologies, LLC, BRIAN JENSEN, KYLE RAMOS, JOHN YEAGER, Los Alamos National Laboratory, KAMEL FEZZAA, APS, Argonne National Laboratory, DAVID ESQUIBEL, National Security Technologies, LLC — The diagnostic needs of any dynamic loading platform present unique technical challenges that must be addressed in order to accurately measure in situ material properties in an extreme environment. The IMPULSE platform (IMPact system for Ultrafast Synchrotron Experiments) at the Advanced Photon Source (APS) is no exception and, in fact, may be more challenging, as the imaging diagnostics must be synchronized to both the experiment and the 60 ps wide x-ray bunches produced at APS. The technical challenges of time-resolved x-ray diffraction imaging and high-resolution multi-frame phase contrast imaging (PCI) are described in this paper. Example data from recent IMPULSE experiments are shown to illustrate the advances and evolution of these diagnostics with a focus on comparing the performance of two intensified CCD cameras and their suitability for multi-frame PCI. The continued development of these diagnostics is fundamentally important to IMPULSE and many other loading platforms and will benefit future facilities such as the Dynamic Compression Sector at APS and MaRIE at Los Alamos National Laboratory.

1 Part of this project was funded by the “Bundesministerium fuer Bildung und Forschung” under contracts 05KSTRF1 and 05K10RFA “Verbundprojekt: Messeinrichtungen fuer die Material- und Strukturforschung an PETRA III, 2: Laserheizung fuer “ECB”

4:00PM E5.00003 Matter in Extreme Conditions (MEC) Instrument at the Linac Coherent Light Source  
HAE JA LEE, LCLS, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — The behavior and physical properties of matter under extreme conditions are of fundamental scientific interest. Extreme conditions created by intense light sources generates dense state with densities of up to several times solid density, temperatures of 10 keV to 100 keV, and pressures of 10s kbar to 100s Mbar. Model calculations in this regime predict electronic and structural phase transitions with new atomic and electronic band structure, anomalous transport, and changes of scattering properties and opacity. A new technique using the Linac Coherent Light Source (LCLS), an x-ray free electron laser laser source, was developed at MEC in Extreme Conditions (MEC) endstation to study wide range of extreme conditions in phase space. The LCLS has >3 mJ per 60 fs pulse enabling an intensity x-ray beam between 4 keV -9.5 keV to be focused onto a small spot ~1 micron at MEC. The research areas that MEC instrument will address include equation of state, behavior of materials under high-pressure, and phenomena of solid materials under extreme conditions. We operate MEC instrument for users’ experiments studying warm dense matter, hot dense matter, and high pressure physics. Here, we present the details of the MEC instrument, capabilities, and progress.

The MEC Instrument is funded by fusion energy science of the U.S. Department of Energy. The author would like to thank the LCLS MECi project team.

4:30PM E5.00004 Time resolved and Extreme conditions X-ray Absorption Spectroscopy (TEXAS) at the European Synchrotron Radiation Facility  
SAKURA PASCARELLI, ESRF — The ESRF has started an ambitious project spread over 10 years aimed at an upgrade of the accelerator, beamlines and infrastructure. One of the first upgrade beamlines (UPBLs) to become operational, UPBL11, is specifically dedicated to Time resolved and Extreme conditions X-ray Absorption Spectroscopy (TEXAS). This facility, based on the upgrade of the former energy dispersive XAS beamline ID24, will provide the user community new opportunities for investigating matter at extreme conditions of pressure, temperature and magnetic field. Target experiments for the future include kinetic studies of chemical reactions at high pressure and temperature, and investigation of extreme states of matter that can be maintained only over very short periods of time. Since UPBL11 has only recently been opened to user operation, I will first give a brief overview of results obtained on the former ID24 in the area of extreme conditions. Examples cover element selective magnetometry under pulsed magnetic fields of 30 T, studies of chemical reactions that occur in the interior of planets, the investigation of pressure induced collapse of ferromagnetism in 3d metals, and first attempts to probe the electronic and local structure in melts at high pressures. Then I will illustrate the status and the performance of the new dedicated experimental setups for extreme conditions on UPBL11. First results from the new laser heating facility able to reach the multi-megabar regime at temperatures above 4000 K and the pulsed high magnetic field facility for XAS studies under fields up to 35 T and temperatures down to 1.5 K will be given. I will conclude with a few ideas for future experiments that exploit the advantages of the energy dispersive optical scheme for the study of matter under conditions so extreme that they can be maintained only for very short periods of time.

5:00PM E5.00005 New Hybrid Experimental Facility for High-Pressure / Low-Temperature XRD at SPring-8  
YASUO OHISHI, NAOHISA HIRAO, Japan Synchrotron Radiation Research Institute (SPring-8), TAKAHIRO MATSUOKA, Messeinrichtungen fuer die Material- und Strukturforschung an PETRA III, DESY — The behavior and physical properties of high-pressure and high-temperature subjects are of fundamental scientific interest. Extreme conditions created by intense light sources generates dense state with densities of up to several times solid density, temperatures of 10 keV to 100 keV, and pressures of 10s kbar to 100s Mbar. Model calculations in this regime predict electronic and structural phase transitions with new atomic and electronic band structure, anomalous transport, and changes of scattering properties and opacity. A new technique using the Linac Coherent Light Source (LCLS), an x-ray free electron laser laser source, was developed at MEC in Extreme Conditions (MEC) endstation to study extreme conditions in phase space. The LCLS has >3 mJ per 60 fs pulse enabling an intensity x-ray beam between 4 keV -9.5 keV to be focused onto a small spot ~1 micron at MEC. The research areas that MEC instrument will address include equation of state, behavior of materials under high-pressure, and phenomena of solid materials under extreme conditions. We operate MEC instrument for users’ experiments studying warm dense matter, hot dense matter, and high pressure physics. Here, we present the details of the MEC instrument, capabilities, and progress.

5:15PM E5.00006 New possibilities at beamline ID27 of the ESRF  
MOHAMED MEZOUAR, GASTON GARBARINO, PARASKEVAS PARIASIDIS, JEROEN JACOBS, STANY BAUCHAU, ESRF — Beamline ID27 is fully optimised for monochromatic high resolution XRD in order to address the most exciting and challenging questions related to science at very high pressures. This beamline can easily accommodate very complex sample environments such as the double-sided laser heating system, the Paris-Edinburgh press and the HP helium cryostat. These techniques are powerful tools to explore a very wide pressure (P>2 Mbar) and temperature domain (5<T<5000 K). The beamline components (source, optics and detectors) are entirely designed to give the best possible response to these very demanding conditions. The most recent developments including an in situ CO2 laser heating system and a high temperature resistively heated diamond anvil cell will be presented.
3:30PM E6.00001 Percolation of Blast Waves though Sand1, WILLIAM PROUD, Institute of Shock Physics, Imperial College London, London, SW7 2AZ, United Kingdom — Previous research has concentrated on the physical processes occurring when samples of sand, of varying moisture content, were shock compressed. In this study quartz sand samples are subjected to blast waves over a range of pressure and duration. Aspects of particle movement are discussed; the global movement of a bed hundreds of particles thick is a fraction of particle width. The main diagnostics used are pressure sensors and high-speed photography. Results are presented for a range of particle sizes, aspect ratio, density and moisture content. While the velocity of the percolation through the bed is primarily controlled by density and porosity the effect of moisture reveals a more complex dependence.

1The ISP acknowledges the support of the Atomic Weapons Establishment and Imperial College London

3:45PM E6.00002 Shock and Release Behaviour of Sand, JAMES PERRY, University of Cambridge — A considerable body of knowledge exists on the shock properties of dry sand. However, capturing the release properties have proven experimentally complex, and currently little information exists on the topic. The measured Hugoniot and release behaviour from a number of experiments is presented, carried out with the aim of furthering or understanding of the fundamental physics behind the unloading of dry sand from a shocked state. Additionally, progress on extending the investigation to sand with varying water content will also be presented.

4:00PM E6.00003 Experiments and Simulation of Split Hopkinson Bar tests on Sand, PHILIP CHURCH, ANDY WOOD, PETER GOULD, QinetiQ, ANDY TYAS, Sheffield University, QINETIQ TEAM2, SHEFFIELD UNIVERSITY TEAM3 — Split Hopkinson Bar data has been generated for well controlled dry and wet sand under confined and unconfined conditions. Simulations have been performed with the Lagrangian hydrocode DYNA using a Porter-Gould Equation of State (EOS) and Johnson-Holmquist type constitutive model. Comparison with the raw strain gauge data is qualitatively reasonable, although some of the details of the trace are not reproduced. This has given some insights into how the constitutive model should be improved.

1Support from UK MoD
2QinetiQ did the modelling
3Sheffield did the experiments

4:15PM E6.00004 Meso-scopic Densification in Brittle Granular Materials, WILLIAM NEAL, Applied Modelling and Computational Group, Imperial College London, GARETH APPLEBY-THOMAS, Dynamic Response Group, Cranfield University, GARETH COLLINS, Applied Modelling and Computational Group, Imperial College London — Particulate materials are ideally suited to shock absorbing applications due to the large amounts of energy required to deform their inherently complex meso-structure. Significant effort is being made to improve macro-scale material models to represent these atypical materials. On the long road towards achieving this capability, an important milestone would be to understand how particle densification mechanisms are affected by loading rate. In brittle particulate materials, the majority of densification is caused by particle fracture. Macro-scale quasi-static and dynamic compaction curves have been measured that show good qualitative agreement. There are, however, some differences that appear to be dependent on the loading rate that require further investigation. This study aims to investigate the difference in grain-fracture behavior between the quasi-static and shock loading response of brittle glass microsphere beds using a combination of quasi-static and dynamic loading techniques. Results from pressure-density measurements, sample recovery, and meso-scale hydrocode models (SALE, an in-house simulation package) are discussed to explain the differences in particle densification mechanisms between the two loading rate regimes.

1Gratefully funded by AWE plc

4:30PM E6.00005 Time Scales in Particulate Systems, DUAN ZHANG, Los Alamos National Laboratory — While there are many interests of studying interactions of individual particles, macroscopic collective behavior of particles are our main interest in many practical applications. In this talk, I will give a brief overview of the multiscale methods connecting the physics at individual particles to macroscopic quantities and averaged equations. The emphasis will be on dense dissipative particulate systems, such as powders. Unlike conservative particle systems, such as molecular systems, in a dissipative particle system the concept of thermodynamic equilibrium is not very useful unless in very special cases, because the only true thermodynamically equilibrium state that exists is the state in which nothing moves. Other than idealized simple systems, mesoscale structures are common and important in many practical systems, especially in dissipative systems. Spatial correlations of these mesoscale structures, such as force chains in dense granular system, particle clusters and streamers in fluidized beds have received some recent attentions, partly because they can be visualized. This talk will emphasize the effects of time correlations related to the mesoscale structures. To consider time correlations and history information of the system, I will introduce the mathematical foundation of the Liouville equation, its applicability and limitations. I will derive the generalized Liouville equations for particulate systems with and without interstitial fluids, and then use them to study averaged transport equations and related closures. Interactions among the time scale of particle interactions, the time scale of the mesoscale structures, and the time scale of the physical problem as represented by strain rate will be discussed. The effect of these interactions on the closure relations will be illustrated. I will also discuss possible numerical methods of solving the averaged equations, and multiscale numerical algorithms bridging the particle level calculations to continuum level calculations.

1This work was sponsored by Stockpile Safety and Surety Program, the Joint DOD/DOE Munitions Technology Development Program, and National Nuclear Security Administrations Science Campaign 2

5:00PM E6.00006 Shock-Induced Deformation in Dry and Wetted Particle Beds, BRADLEY MARR, OREN PETEL, DAVID FROST, ANDREW HIGGINS, McGill University, Department of Mechanical Engineering, Montréal, QC, H3A 0C3, Canada — The high strain rate response of granular media has received considerable attention due to increasing interest in granular penetration. It has been shown under high-rate dynamic loading dry sand particles undergo a transition in the dominant mechanism of global deformation of the particle bed from a response governed by particle slippage to one governed by particle deformation. In the present study, we investigate the response of packed particle beds, both wetted and dry, under varying flyer plate induced shock loadings. We investigate the critical conditions for the onset of particle deformation in systems of spherical macroscopic particles of various materials. Resulting particle deformations from the shock compression are characterized using scanning electron microscopy with the recovered samples, and the effects of shock strength, particle size, and particle material properties are compared.
The Role of Intrinsic Material Properties on Shock-Induced Sliding

MARK COLLINSON, DAVID CHAPMAN, DANIEL EAKINS, Institute of Shock Physics, Imperial College London — The high strain-rate behaviour of multi-component systems is often dominated by mediation at material interfaces. The extent to which a material’s microstructure influences dynamic friction and relative sliding response remains an area of active study. We present results of a recent study into the behaviour of dry metallic interfaces under the passage of a controlled loading wave. The role of material strength linked to grain size and precipitates have been investigated through experiments on stainless steel and aluminium components of varying alloy composition and microstructure. Held in close contact along a single planar interface, oblique shock waves were generated along this boundary by direct copper flyer impact at velocities in the range 250 m/s - 600 m/s. Both the 100mm and 13mm bore gas guns located at Imperial College London were utilised for this purpose. Multiple channels of frequency shifted PDV were employed to measure the individual far field responses of the specific materials, while a line-imaging VISAR system was used to directly record the velocity profile across the contact interface, providing a measure of any spatially dependent response. Comparisons of these results against current generation hydrocode models are presented, with good agreement attained with PDV measurements in the far field.

Monday, July 8, 2013 3:30PM - 5:15PM –
Session E7 CH.2 Chemistry: Complex Molecules Grand Crescent - Dana Dlott, University of Illinois

Probing Physical and Chemical Properties of Laser Shocked Materials using Ultrafast Dynamic Ellipsometry and Spectroscopies

NHAN DANG, Los Alamos National Laboratory — Ultrafast laser techniques allow resolution of shock-induced physics and chemistry picoseconds behind the shock front. In this presentation, the 350 ps sustained laser-generated shocks will be shown to combine with ultrafast dynamic ellipsometry to measure the shock state and transient absorption to measure the molecular electronic response to shock loading. Experimental data will be presented on shocked explosive crystals and liquids. Ultrafast dynamic ellipsometry was used to measure the shock and particle velocity as well as the shocked refractive index. Transient absorption spectra of RDX and simple molecular liquids in the spectral region from 440 to 780 nm were measured to map out shock reactivity during the first 350 ps, over shock stress states from 7 to 20 GPa. Additionally, nonlinear spectroscopic probes will be demonstrated to offer the potential to measure even more details of the molecular shock response, such as evolution of chemical species and vibrational temperature. Preliminary results of shocked phenylacetylene obtained using vibrational coherent anti-Stokes Raman spectroscopy (CARS) and the capability of femtosecond stimulated Raman scattering (FSRS) data to measure the nonequilibrium time evolution of mode specific vibrational temperatures on picosecond time scales will be discussed.

Shock-driven chemical reaction in phenylacetylene

DANA DATTLEBAUM, STEPHEN SHEFFIELD, JOSHUA COE, Los Alamos National Laboratory, SHOCK AND DETONATION PHYSICS TEAM, PHYSICS AND CHEMISTRY OF MATERIALS TEAM — Phenylacetylene (PA) comprises a covalently-linked benzene ring and acetylene moiety, presenting an interesting molecular structure for study of shock driven chemical reactions. In the present work, gas gun-driven embedded electromagnetic gauging experiments produced in situ particle velocity wave profiles at multiple Lagrangian positions at several shock input conditions. The input shock wave evolves over time and distance into a complex multiple wave structure, with a fast risetime 2nd wave, slower risetime 3rd wave, and unusual wave dynamics in the 1st wave. From the shock and particle velocities, the Hugoniot reaction condition, and intermediate and final states associated with the chemical reactions have been obtained. For example, at shock inputs just above the cusp condition, an induction time of 200 ns was observed, with the evolved first wave traveling at $u_0 = 4.2 \text{ km/s}$, $P = 5.6 \text{ GPa}$; reaction rates of a few to 10 microsec$^{-1}$ were inferred. A thermodynamically complete unreacted equation of state was calibrated to estimate the temperature rise along the shock locus. Use of this EOS with the measured wave risetimes yielded highly state-sensitive global reaction rates.

Observations on shock induced chemistry of cyclohexane

MINTA AKIN, RICKY CHAU, Lawrence Livermore National Laboratory — We use double pass absorption spectroscopy to examine shock induced reactions in situ in cyclohexane and benzene at pressures up to 33.1 GPa. Reactions in cyclohexane begin by 27 GPa and complete by 33.1 GPa. Absorption spectra indicate that the first reaction occurs within or near the shock front, and that a metastable local equilibrium is reached in the post-shock state. A second process is observed upon reschock at the lower pressures, suggesting a new equilibrium is reached post-reschock as well. Absorption bands are consistent with the formation of short radicals or fragments upon decomposition; however, spectral resolution is too low to confirm this mechanism. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Induced Phase Transitions of Cycloheptanone and Cycloheptanol up to 30 GPa

CHUNLI MA, QILIANG CUI, Jilin University, ZHENXIAN LIU, Carnegie Institution of Washington — High-pressure spectroscopic studies of cycloheptanone (C7H12O) and cycloheptanol (C7H14O) have been carried out up to 30 GPa at room temperature using Raman scattering and infrared absorption combined with diamond anvil cell techniques. Different phase transition behaviors in these derivatives of cycloheptane have been observed. Both Raman and infrared absorption spectra show dramatic changes at 1 GPa including the appearance of new peaks and peak sharpening/splitting. These changes can be attributed to the phase transition from liquid phase into true crystalline phase. With further compression, cycloheptanone gradually turns into amorphous state when pressure higher than 24.0 GPa. In contrast, no truly crystalline phase was observed in cycloheptanol up to 30 GPa. A phase transition from liquid to plastic phase was observed around 1.5 GPa based on the synchrotron angle dispersive x-ray diffraction measurements. The cycloheptanol begins to transform into glass phase around 4.0 GPa as all the Raman, infrared and x-ray diffraction peaks start to broaden. The mechanism of very different phase transitions presented in these derivatives of cycloheptane with two different substituent groups has been discussed.

High Pressure Raman Spectroscopy of Hydrogen Bonded, Layered Crystal of Squaric Acid

ZBIGNIEW DREGER, JUEFEI ZHOU, YUCHUAN TAO, YOGENDRA GUPTA, Washington State University — High pressure Raman spectroscopy experiments were carried out on squaric acid (H$_2$C$_2$O$_4$) to understand the role of hydrogen bonding on the structural and chemical stability of layered molecular crystals. Measurements in a diamond anvil cell (up to 70 GPa) revealed several instances of structural changes: (1) disappearance of some lattice modes at 0.6-0.9 GPa, indicating a change in the crystal structure symmetry from monoclinic to tetragonal, (2) disappearance of some intramolecular modes at 3 GPa, indicating possible symmetrization of hydrogen bonding in crystal layers, and (3) appearance of new intramolecular modes at 13-14 GPa. The latter changes were accompanied by a gradual increase in the Raman intensity and changes in the widths of lattice and intramolecular modes. No chemical changes were observed over the pressure range examined. These results suggest that hydrogen bonding network in layers is preserved to the highest applied pressures. However, the layers could be distorted with respect to each other above 13 GPa. Work supported by DOE/NNSA and ONR/MURI.
5:00PM E7.00006 High-Pressure Effects in Benzoic Acid Dimers: Vibrational Spectroscopy, YUCHUAN TAO, ZBIGNIEW DREGER, YOGENDRA GUPTA, Washington State University — To understand pressure effects on dimer structure stability, Raman and FTIR spectroscopy were used to examine changes in hydrogen bonded dimers of benzoic acid crystals up to 31 GPa. Raman measurements indicated a phase transition around 7-8 GPa. It is proposed that this transition is caused by a rearrangement of molecules within the dimer leading to a symmetry change from C_{2v} to either C_{2} or C_{s}. This change was reversible upon pressure release from 15 GPa. Pressures above 15 GPa induced gradual changes in luminescence and color change in the crystal. FTIR measurements at 31 GPa revealed the formation of a new broad band centered around 3250 cm\(^{-1}\), which was attributed to the stretching vibrations of the O-H bond. It is proposed that hydrogen bonded dimers of benzoic acid transform partially to a covalently bonded compound composed of benzoic anhydride-like molecules and H\(_2\)O. This study demonstrates that application of high pressure can lead to significant changes in the H-bonded dimer structure, including formation of chemical bonding. Work supported by DOE/NNSA and ONR/MURI.

5:30PM - 5:30PM
Session F1 Poster Session I (5:30 - 7:00PM) Grand Ballroom I

F1.00001 Raman Spectroscopy of Tin Monoxide under High Pressure, REUBEN SHUKER, ASAF PESACH, Ben Gurion University, Beer Sheva, Israel, RAMAN LABORATORY TEAM — Under ambient conditions, tin monoxide crystallizes in litharge structure which consists of tetragonal P4/nmm symmetry. An orthorhombic distortion of this compound at high pressure is assumed to be driven by softening of the unobserved $B_{1g}$ phonon, which results in a spontaneous strain in the xy plane of the tetragonal unit cell. In this case, a reduction of the symmetry into Pm$\bar{3}$m occurs. The correlation between the tetragonal and orthorhombic symmetries shows a splitting of the degenerated $E_g$ phonon into a superposition of $A_1$ and $B_1$ phonons in the lower symmetry. This splitting was observed in our pressure dependent Raman scattering measurements. The changes in the pressure induced Raman spectrum of tin monoxide can be quantitatively obtained by first order perturbation theory. The frequency of this phonon under stress is obtained by diagonalizing the relevant matrix. This procedure gives a frequency shift and splitting of $E_g$ phonon as a function of pressure induced strain. By means of Landau’s classical free energy theory this order parameter gives a critical pressure value of 1.03 GPa for the phase transition.

F1.00002 Attempts in PTTT diagram of pressure induced phase transformations, S.M. HONG, X.R. LIU, L.Y. CHEN, Z. HE, D.D. ZHANG, M.Y. WANG, C.R. ZHANG, Laboratory of High Pressure Physics, Southwest Jiaotong University, China — Temperature-time-transition (TTT) diagram is widely applied for understanding the kinetic behavior of temperature induced phase transition. In contrast to it, kinetic behavior of pressure induced phase transitions is still not effectively researched, although many equilibrium phase diagrams have been found up to very high pressure. In fact, behavior of diamond nucleation and growth from C-H-O system could be well known through characterization of recovered samples. The results suggest time-dependent conditions of pressures and temperature. A notional kinetic phase diagram is established by previous experimental and geological data. In recent years, we made a pressure-jump apparatus with the compression rate from several to 500GPa/s within 100GPa, such rate range lies in the gap between conventional static and dynamic high pressure experiments. By using it, some novel metastable phases were solidified through rapid compressing their melts, including alloys, non-metallic elements and polymers. Comparing characterization of recovered phases with the experimental conditions, dependence of phase transition on the compression rates could be clearly demonstrated, furthermore, combining with heating or cooling rates at high pressure, the kinetic phase diagram with three dimensions, pressure, temperature and time, (PTTT diagram) could be established.

F1.00003 Observation of electrical and magnetic property of CaRhO$_3$ and CaRhO$_3$ post-perovskite by electrical resistivity measurement under high pressure, KOTA ICHIMARU, KENJI OHTA, KATSUYA SHIMIZU, KYOKUGEN, Osaka University, Japan, KENYA OHGUSHI, ISSP, University of Tokyo, Japan, KAZUNARI YAMAURA, NIMS, Japan — Since discovery of MgSiO$_3$ post-perovskite (PPv) phase, high-pressure polymorph of MgSiO$_3$ perovskite (Pv), there are extensive studies regarding physical properties of various PPv materials. It is well known that the crystal structure of high-Tc cuprates is based on Pv structure. Material with PPv structure is thus expected to show superconducting behavior with high $T_c$. Here we investigated electrical properties of CaRhO$_3$ and CaRhO$_3$ PPv. These PPv materials are quenchable to ambient condition, and known as a quasi-2D Mott Insulator showing antiferromagnetic transition at low temperature [1,2]. We performed electrical resistivity measurements on the samples under high pressure and low temperature conditions up to 191 GPa, and found that the energy gap of both samples came close to zero with applying pressure. On CaRhO$_3$ PPv, we observed an abrupt increase in sample resistivity at low temperature, which is likely to correspond to antiferromagnetic transition in the same material. FTIR measurements at 31 GPa revealed the formation of a new broad band centered around 3250 cm\(^{-1}\), which was attributed to the stretching vibrations of the O-H bond. It is proposed that hydrogen bonded dimers of benzoic anhydride-like molecules and H\(_2\)O. This study demonstrates that application of high pressure can lead to significant changes in the H-bonded dimer structure, including formation of chemical bonding. Work supported by DOE/NNSA and ONR/MURI.

F1.00004 Presence of paramagnetism in HoCo$_2$ under hydrostatic pressure, JAROSLAV VALENTA, JIRI PRCHAL, MARIE KRATOCHVILA, MARTIN MISEK, VLADIMIR SECHOVSKY, Charles University in Prague, DCMP, CHARLES UNIVERSITY IN PRAGUE, DCMP TEAM — HoCo$_2$ belongs to a group of RECo$_2$ compounds (RE = rare earth metal) which were previously studied mostly due to presence of two types of magnetism - the localized RE magnetic moment and the Co moment originating in the splitting of the Co 3d subbands. The corresponding RE and Co magnetic sublattices are both ferromagnetic and antiparallel to each other for RE $\in$ (Gd..Tm) below $T_C$. In 2007 Herrero-Albillos et al. published experimental evidences of the Co moments surviving in paramagnetic state above $T_1$ in ErCo$_2$. The surviving Co magnetic moments form small (ferromagnetic) clusters coupled antiparallel to the nearest RE magnetic moments in the paramagnetic state. These antiparallel short-range Co-Cr moment correlations at $T > T_C$ are denoted as paramagnetism. Above a characteristic temperature $T_J$ (observed in the AC magnetic susceptibility data as a tiny anomaly) the Co magnetic moment turns to the same direction as Er magnetic moment. The phenomenon of paramagnetism has been recently confirmed for HoCo$_2$. In 2011 Bonilla at. al. presented results from $\mu$ SR experiment on ErCo$_2$. Results of the $\mu$ SR experiment show the presence of Co magnetic clusters up to temperature $T > T_J$. We present experimental results AC susceptibility measurements for HoCo$_2$ under hydrostatic pressure up to 3 GPa and $\mu$ SR data under hydrostatic pressure up to 2 GPa. The results will be discussed in terms of corresponding variations of the hierarchy inter- and intra-sublattice exchange interactions.

F1.00005 Vibrational properties of Ba$_2$Ga$_{14}$Sn$_{30}$ under high pressure, TATSUO SUKEMURA, TETSUJI KUME, SHIGEO SASAKI, Gifu University, TAKAHIRO ONIMARU, TOSHIRO TAKABATAKE, Hiroshima University — Semiconductor clathrates consist of host cages made by group-14 (13 and 15) atoms with sp$^3$ network, and guest atoms encapsulated into the host cages. Ba$_2$Ga$_{14}$Sn$_{30}$ clathrate are well known to provide a typical rattling vibration of the guest. Because of the cage size much larger than guest ion size, the guest ions are located not at the center of the cage, leading to so-called off-center rattling vibration. The sizes of guest ion and/or host cage are important for the rattling nature. It is straightforward to apply the pressure for investigate the rattling vibration which is expected to be highly sensitive to the host cage size. In this paper, we provide the dependence of the rattling vibration of Ba$_2$Ga$_{14}$Sn$_{30}$ on the pressure.

Great thanks to the National Natural Science Foundation of China (10774123 and 11004163) for financial support.

F1.00006 High pressure melting of Tellurium, RAN SALEM, NRCN, SHLOMI MATITYAHU, Ben Gurion University, ORI NOKE, AVIVA MELCHIOR, ERAN STERER, NRCN — The melting curve of Tellurium was measured in a laser heated diamond anvil cell (LHDAC). Using our IR pyrometer we were able to measure melting temperatures as low as 600 K. Melting at high-pressure was identified by image analysis of an auxiliary laser light scattering images, taken from the surface of the hot spot, and designed to detect changes in the sample surface due to melting. Our data is consistent with previous measurements performed in a large volume press and go to higher pressure.

F1.00007 Application of the shock reverberation technique to determine Grüneisen gamma for float glass, MICHAEL GIBSON, GARETH APPLEBY-THOMAS, ANDREW ROBERTS, Cranfield University, PAUL HAZELL, University of New South Wales — Determination of high strain-rate material properties following loading from a non-principle Hugoniot ground state requires detailed knowledge of the shape of a materials equation-of-state. The material-specific variable Grüneisen gamma, $\gamma(v)$, defines the shape of ‘off-Hugoniot’ points in energy-volume-pressure space. Comparison between experimental and simulated results of ‘ring-up’ experiments, where shock reflection allows a material to be loaded successively into a series of ‘off-Hugoniot’ states, has the potential to allow ready access to values of $\gamma$. However, previous attempts to determine $\gamma$ via comparison to ANSYS Autodyn$^\text{®}$ simulations for the temperature-resistant polymer polyether ether ketone (PEEK) only produced a partial success, due to the highly non-linear nature and poorly defined residual deviatoric (strength) effects inherent in the material response. Consequently, in this study an attempt is made using a similar approach to calculate $\gamma$ for the well-defined material float glass (whose high elastic limit should also minimise deviatoric effects).

F1.00008 Modeling Dynamic Compaction of Porous Materials with the Overstress Approach, YEHUDA PARTOM, Retired — To model compaction of a porous material (PM) we need 1) an equation of state (EOS) of the PM in terms of the EOS of its matrix, and 2) a compaction law. For the EOS it is common to use Herrmann’s suggestion, as in his $P\alpha$ model. For a compaction law it is common to use a quasi-static compaction relation obtained from 1) a mezzo-scale model (as in Carroll and Holt’s spherical shell model), or from 2) quasi-static tests. Here we are interested in dynamic compaction, like in a planar impact test. In dynamic compaction, the state may change too fast for the state point to follow the quasi-static compaction curve. We therefore get an overcompaction situation. The state point moves out of the quasi-static compaction boundary, and only with time collapses back towards it at a certain rate. In this way the dynamic compaction event becomes rate dependent. In the paper we first write down the rate equations for dynamic compaction according to this overcompaction approach. We then implement these equations in a hydro-code, and run some examples. We show how the overcompaction rate parameter can be calibrated from tests.

F1.00009 Shock-recovery studies on InSb single crystals up to 24 GPa, HIROAKI KISHIMURA, HITOSHI MATSUMOTO, Department of Materials Science and Engineering, National Defense Academy — A series of shock-recovery experiments on InSb single crystals along the (100) or (111)-axis up to 24 GPa were performed using a flyer plate impact. The structures of recovered samples were characterized by X-ray diffraction (XRD) analysis. According to calculated peak pressures and temperatures, and phase diagram for InSb, the sample could undergo phase transitions from zinc-blende structure to high-pressure phases. However, the XRD trace of each sample revealed the absence of additional constituents including metastable phases and high-pressure phases of InSb except for 15 and 16 GPa. The XRD trace of each sample corresponded to powder pattern of InSb with zinc-blende structure. At 16 GPa, in addition to zinc-blende structure, additional peaks were obtained. One of these peaks may correspond to the $Cmcm$ or $Immm$ phase of InSb, and the other peaks were not identified.

F1.00010 The evolution of bulk strength behind a shock propagating in metals with controlled flaw populations, CHRISTOPHER SHEPHERD, The University of Kent, GARETH APPLEBY-THOMAS, Cranfield University, NEIL BOURNE, AWE, DAVID WOOD, Cranfield University, JEREMY MILLETT, AWE — Plastic deformation in metals in the “weak shock” regime occurs by slip in the metals crystaline structure. However, such atomic motions take a finite time. Consequently, coalesce of inherent flaws leading to a macroscopic compressive strain will not occur immediately on shock arrival. In this study the effect of artificially induced flaws in the well-characterised FCC metal Al on strength behind the shock was interrogated. Cold-pressing of two differing particle size/morphology plasma-spray powders to close to bulk density allowed generation of microstructures with inherent flaws on the initial powder-size scale. Inclusion of longitudinal and lateral Manganin stress gauges then allowed the temporal evolution of material shear strength to be monitored at different distances from the impact face. Comparison to the response of bulk material subsequently allowed de-convolution of the influence of the induced flaws in the pressed structures.

F1.00011 Plate impact experiments and simulation on porous graphite, DAVID HEBERT, GABRIEL SEISSON, ISABELLE BERTRON, JEAN-MARC CHEVAILIER, CHRISTIAN THESIEUX, JEAN-HUGUES QUESADA, STEPHANIE TASTET, CEA — We present some plate impact experiments on a commercial grade of graphite. The dynamic loadings range between 0.4 and 15 GPa under shock, and reach 25 GPa under reshock in the samples, which were approximately 20% porous and macroscopically isotropic. Material velocity at the sample rear surface is measured and recorded optically with Visar or Perret-Fabry interferometers. These experimental results are then compared to hydrodynamic simulations. The model for graphite takes porosity into account, and the parameter fitting will be presented. Our model is also compared to previously published experimental data. The overall agreement is good.

F1.00012 The $\alpha\rho\lambda$-model of Operational EoS, MICHAEL GRINFELD, The U.S. Army Research Laboratory — The operational EoS concept can be traced back to fundamental principles of thermodynamics. From the one hand, the operational EoS is nothing else but the complete EoS, i.e., one of the thermodynamic potentials referred to their canonically adjoint thermodynamic variables. On the other hand, the operational EoS is the operator (typically, integro-differential operator) of the measured series of experimental data. The dynamic loadings range between 0.4 and 15 GPa under shock, and reach 25 GPa under reshock in the samples, which were approximately 20% porous and macroscopically isotropic. Material velocity at the sample rear surface is measured and recorded optically with Visar or Perrot-Fabry interferometers. These experimental results are then compared to hydrodynamic simulations. The model for graphite takes porosity into account, and the parameter fitting will be presented. Our model is also compared to previously published experimental data. The overall agreement is good.

F1.00013 Effect of Pressure on Some Optical Properties of Ga$_{1-x}$In$_x$P Semiconductors, P.S. VYAS, V. P. & R. P. T. P. Science College, P.N. GAJJAR, Gujarat University, A.R. JANI, Sardar Patel University — A theoretical procedure is presented for the study of optical properties of ternary alloy Ga$_{1-x}$In$_x$P. The calculations are based on the pseudopotential formalism in which local potential coupled with the virtual crystal approximation (VCA) is applied to evaluate the effect of pressure on the optical properties like refractive index, electronic polarizability, plasmon energy, dielectric constant and equation of state for gallium concentration $x = 0, 0.25, 0.50, 0.75$ and $1$ of the ternary alloy Ga$_{1-x}$In$_x$P. To incorporate the screening effect, local field correction functions due to Hartree, Taylor, Ichimaru et al. and Nagy are employed. The refractive index, electronic polarizability and dielectric constant computed for the parent binary compounds GaP and InP are found to be satisfactorily agreeing with the experimental report. It is seen that the refractive index of Ga$_{1-x}$In$_x$P decreases nonlinearly with the increase in pressure. The results obtained using Hartree’s screening functions are not very close to the experimental data as it does not include any exchange and correlation effects. Overall good agreement with the experimental and other theoretical findings confirms the application.

$^1$The author P. S. Vyas is thankful to UGC, New Delhi, India for providing financial support under minor research project No. F.: 47-651/08(WRO).
F1.00014 Structural, electronic and phase transition properties of ytterbium monopnictides under high pressure: A LSDA+U study1, SANJAY KUMAR SINGH, P. RANA, U.P. VERMA, School of Studies in Physics, Jiwaji University, Gwalior-474011, Madhya Pradesh, India — In present paper, we have investigated the structural, electronic properties of ytterbium monopnictides (YbX = N, P) and its phase transition behaviour under high pressure by using the full potential linear augmented plane wave plus local orbitals approach within the framework of density functional theory. In the study the generalized gradient approximation (GGA) is chosen for the exchange-correlation functional energy. The equilibrium properties viz., equilibrium lattice constants, bulk modulus, its pressure derivative and total energy are calculated in four different phases i.e. B1, B2, B3 (zinc blende), and BCT phases and compared with previous calculations and available experimental data. The local spin-density approximation along with Hubbard-U corrections and spin-orbit coupling has been used for correct prediction of electronic properties. The LSDA + U strategy shows significant impact on the energy levels of the occupied and unoccupied 4f states in the electronic structure of both the compounds. The calculation shows YbX to be semi-metallic. The LSDA + U method provides better description of crystal properties of present system. At ambient conditions YbX (X = N, P) stabilize in NaCl (B1) structure characterized by the space group Fm-3m. Under compression, both YbN and YbP undergo first-order structural transition from Fm-3m (B1) to Pm-3m (B2) at 164.0 and 31.0 GPa, respectively.

1The One of the authors (UPV) acknowledges the financial assistance provided by UGC, New Delhi F. no. 36-124/2008(SR), India.

F1.00015 The dehydration of potassium alum induced by shock loading , HIROAKI KISHIMURA, YUHATA IMASU, HITOSHI MATSUMOTO, Department of Materials Science and Engineering, National Defense Academy — Shock-induced dehydration and structural change on potassium alum, Ka(SiO2)2·12H2O, has been studied up to a peak pressure of 8 GPa. The shock-recovered samples have been characterized using Raman spectroscopy, x-ray diffraction (XRD), and a scanning electron microscopy (SEM). Although the sample shocked at 5 GPa are consolidated and recovered, no evidence for structural change or dehydration is obtained. However, prominent change of texture and color of the recovered sample shocked at 8 GPa is observed. The XRD results reveal that the recovered sample shocked at 8 GPa consists of anhydrous potassium alum crystals with amorphous. This structure differs from that of dehydrated alum caused by heat. The critical pressure for the shock-induced phase transition is close to the transition pressure from alum crystal to amorphous phase, which is obtained by static pressure loading.

F1.00016 Magnetoresistance and electrical properties of multi-component copper chalcogenides at pressures up to 50 GPa , NINA MELNIKOVA, ALEXANDER TEBENKOV, ALEXEY BABUSHKIN, KIRILL KUROCHKA, Ural Federal University, PHASE TRANSITIONS TEAM, TRANSPORT PROPERTIES TEAM, NOVEL MATERIALS TEAM — Multi-component copper chalcogenides based on layered semiconductors A1-B1 (such as InS, InSe, GaS, GaSe, etc.) are new objects of study, they have interesting physical properties and undergo temperature and baric phase transitions. This paper presents the results of a study of the electrical properties and magnetoresistance of CuInS2, CuInSe2, CuInAs2S4, CuInAs2S3, CuInSe2S3 at pressures up to 50 GPa. High pressures have been generated in the cell with synthetic carbonado-type diamond anvils that can be used as electric contacts [1]. Electric properties at high pressure have been investigated on dc current and by means of impedance spectroscopy. Magnetoresistance has been measured in transverse magnetic field. The pressure ranges of noticeable changes in a behavior of magnetoresistivity, of impedance and admittance, tangent of loss angle, relaxation time upon a pressure increase and a pressure decrease are established. This behavior of physical parameters can be due to structural transitions and due to a change of electron structure. This work was supported in part by the Russian Foundation for Basic Research, project no. 13-02-00633.


F1.00017 High-pressure studies of cycloheptane up to 30 GPa1, CHUNLI MA, QILIANG CUI, Jilin University, ZHENXIAN LIU, Carnegie Institution of Washington — High-pressure synchrotron angle dispersive x-ray diffraction, Raman scattering and infrared absorption studies have been performed on cycloheptane (C7H14) up to 30 GPa at room temperature by using diamond anvil cell techniques. The synchrotron x-ray diffraction results indicate that the liquid cyclopentane undergoes two phase transitions at around 0.5 and 1.0 GPa, respectively. Then, it gradually turns into glass state starting from 3.0 GPa. The features of the Raman scattering and infrared absorption show no significant changes with increasing pressure below 3 GPa. This implies that the two phases observed by the x-ray diffraction can be attributed to plastic phases in which the cycloheptane molecules are held in an ordered structure while the molecular orientation is disordered. Up on further compression, all Raman and infrared bands begin broadening around 3.0 GPa that provide further evidence on the transition to glass state. Our results also suggest different paths on phase transitions under isothermal compression at room temperature compare to that previously reported under isobaric cooling at ambient pressure.

1This work was supported by the NSF of China (91014004, 11004074,11074089), the specialized Research Fund for the Doctoral Program of Higher Education (20100111120093), and the National Basic Research Program of China (2011CB808200).

F1.00018 Phase transition criterion under pressure and shear loading1, ZHIPING TANG, YANGBO GUO, Univ. of Sci. and Tech. of China — Does the shear stress affect the transition pressure threshold? It is a question in shock dynamics field. We established the criterions for both “stress induced” and “strain induced” phase transitions under pressure and shear loading. The critical surface in the principal stress space is in-symmetric to the tension and compression and appears to be a conic surface. The effects of pressure, shear stress and temperature on the phase transition are discussed. Since the cylindrical yield surface may intersect with the conic critical surface of phase transition in the principal stress space, it means a “strain induced” phase transition might become a “stress induced” phase transition at certain condition. The prediction is in good agreement with the experiment results.

1Supported by the Chinese National Natural Science Foundation (11072240)

F1.00019 Recording of Phase Transition in Tin in Shock and Release Waves Using Laser Interferometry, STANISLAV FINYUSHIN, ALEXEY FEDOROV, ANATOLIY MIKHAILOV, DMITRIY NAZAROV, EVGENIY CHUDAKOV, DENIS KALASHNIKOV, IVAN TRUNIN, IRINA TERESHKINA, No Affiliation — In this paper the authors present results of experiments, concerning the recording of free surface velocity and particle velocity of tin/Lif window interface of tin sample at the dynamic pressure in the range 10 to 70 GPa, using laser interferometry methods Fabry-Perot and PDV. The features of recorded velocity histories interpreted the polymorphous transitions (the direct β → γ phase transition, the reverse γ → β phase transition) and some points on tin melting curve. The tin samples were loaded by impactor accelerated by explosion products of HE cartridge (the wave with the rectangular profile) or by direct detonation wave of HE layer (the wave with the decaying profile). With the help of PDV method, velocity of particles cloud was recorded with the free surface velocity at the moment when the shock wave front arrived to the tin free surface with the pressure amplitude of P ≥ 19 GPa. This should be corresponding to the liquid-solid phase at the release wave. The tin melting in the shock wave is recorded at the loading pressure of P ≥ 51 GPa. The pressure and temperature numerical simulations were performed for shock compression and the further releasing of tin.
F1.00020 Boron and aluminum halides under pressure - polymerization and chemical transformations, YANSUN YAO, University of Saskatchewan — High-pressure phase transitions of boron and aluminum halides have been theoretically studied. At low pressure, crystals of the familiar monomers (BX₃) and dimers (Al₂X₆) are the structures of choice. While the higher oligomers as well as three dimensional infinite polymers are unstable at ambient pressure, they are stabilized by application of external pressure, taking advantage of the extra orbitals made accessible by the increased coordination. Several new crystal structures of boron and aluminum halides have been predicted at high pressures. Calculated x-ray diffraction patterns and Raman spectra of these phases are in good agreement with available experimental data.

F1.00021 A reversible pressure-induced phase transition in sulfamide, KAI WANG, BO ZOU, Jilin University, STATE KEY LABORATORY OF SUPERHARD MATERIALS TEAM — Sulfamide is a good case of hydrogen bonding networks with the molecular structure H₂NSO₂NH₂. At ambient conditions, sulfamide crystallizes into an orthorhombic structure with the Fdd₂ space group. In this work, powder samples of sulfamide have been studied by Raman spectroscopy and synchrotron X-ray diffraction in a diamond anvil cell up to pressures of 16 GPa. The abrupt changes in Raman spectra around 5 GPa have provided convincing evidence for pressure-induced structural phase transition. This phase transition was confirmed by angle dispersive X-ray diffraction (ADXRD) experiments. On release of pressure, the observed transition was completely reversible with pronounced hysteresis. We propose that this phase transition was due to the rearrangements brought about by changes in the hydrogen bonding networks.

F1.00022 Particle Velocity Fluctuations and Pressure Induced Phase Transitions in Bismuth, ROGER MINICH, FRED STREITZ, RICKY CHAU, DANIEL ORLIKOWSKI, LLNL — The dynamical behavior of a pressure induced phase transitions at high pressures is of current interest in high-pressure physics. It is known that hysteresis plays a major role in most rate driven phase transitions. The area and amplitude of the hysteretic cycle typically exhibit well defined scaling. We have studied the particle velocity correlations in Bismuth samples that have been shock loaded in plate impact experiments with pressures ranging from 3.1 - 14.4 GPa. The data show both global scaling of transition times with pressure as well as local scaling of fluctuation frequency with local average pressure. Using wavelet analysis and temporal autocorrelation functions, the analysis suggests that the phase transition proceeds by a sequence of hysteretic cycles. The onset of the new phase occurs when enough hysteretic cycles result in a sufficiently high phase fraction. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 Lawrence Livermore National Security, LLC.

F1.00023 Toward a Multi-scale Phase Transition Kinetics Methodology: From Nonequilibrium Statistical Mechanics to Hydrodynamics, JONATHAN BELOF, DANIEL ORLIKOWSKI, CHRISTINE WU, Lawrence Livermore National Laboratory, KEITH MCLAUGHLIN, University of South Florida — Shock and ramp compression experiments are allowing us to probe condensed matter under extreme conditions where phase transitions and other non-equilibrium aspects can now be directly observed, but first principles simulation of kinetics remains a challenge. A multi-scale approach is presented here, with nonequilibrium statistical mechanical quantities calculated by molecular dynamics (MD) and then leveraged to inform a classical nucleation and growth kinetics model at the hydrodynamic scale. Of central interest is the free energy barrier for the formation of a critical nucleus, with direct NEMD presenting the challenge of relatively long timescales necessary to resolve nucleation. Rather than attempt to resolve this mechanism, the methodology developed here is built upon the non-equilibrium work theorem [Jarzynski, Phys. Rev. Lett., 78:2690 (1997)] in order to bias the formation of a critical nucleus and thus construct the nucleation and growth rates. Having determined these kinetic terms from MD, a hydrodynamics implementation of Kolmogorov-Johnson-Mehl-Avrami (KJMA) kinetics and metastability is applied to the dynamic compressive freezing of water and compared with recent ramp compression experiments [Dolan et al., Nature (2007)].

F1.00024 Cold compressed graphite – A revisit, YUE MENG, HPCAT, Carnegie Institution of Washington, PRZEMEK DERA, GSECARS, University of Chicago and Hawaii Institute of Geophysics and Planetology, University of Hawaii, GUOYIN SHEN, HPCAT, Carnegie Institution of Washington — Phase transition in cold compressed graphite has been a paradox for several decades. Although a pressure-induced phase change is certainly supported by several lines of experimental evidence, the nature of the change as well as the pressure range of the transition remain unsettled. X-ray diffraction studies have revealed a graphite to hexagonal diamond transition in the pressures from 11 to 25 GPa [1] and recently a graphite to M-carbon transition from 19 to 37 GPa [2]. A transition from graphite-like carbon to an amorphous state was reported based on Raman observations [3]. Several post-graphite structures have also been predicted in recent theoretical studies [4,5]. Here we report x-ray diffraction studies on cold compressed polycrystalline and single crystal graphite samples to above 30 GPa. Instead of the transformation to the hexagonal diamond or M-carbon, we observed a transition from graphite to an amorphous carbon. Our results together with the previous studies point to the importance of the starting material characterization, as well as pressure environment control in the study of phase transition in cold-compressed graphite.


F1.00025 High Pressure Studies on (111)-Terminated CeO₂ Nano-Octahedrons: The Major Effect of Non-Hydrostatic Conditions, LIU BO, LI QUANJUN, LIU RAN, YAO MINGGUANG, LIU BINGBING, State Key Laboratory of Superhard Materials, Jilin University — The effect of nonhydrostatic conditions on high pressure phase transition on (111)-terminated CeO₂ nano-octahedrons were studied using in situ high-pressure Raman spectroscopy. Under non-hydrostatic conditions (with no pressure medium) the CeO₂ nano-octahedrons underwent a reversible phase transition from fluorite phase to α-PbCl₂ phase at 26 GPa, which is lower than the bulk counterpart. In contrast, in our previous research, the CeO₂ nano-octahedrons under hydrostatic conditions are shown to be more stable than the bulk, which is driven by lower compressibility of the exposed (111) planes. The transition pressure from cubic to orthorhombic phase is approximately 3 GPa higher than bulk materials. Further analysis shows that lager stress existing in the grain boundaries is believed to major factor to reduce the phase transition under non-hydrostatic conditions.
F1.00026 A possible existence of phase change of deuterated ice VII at about 11 GPa by X-ray and Raman studies, HISAOKO HIRAI, HIROKAZU KADOBAYASHI, Geodynamics Research Center, Ehime University, TAKAHIRO MATSUOKA, KYOKUGEN, Osaka University, YASUO OHISHI, Japan Synchrotron Radiation Research Institute, TAKEHIKO YAGI, Geodynamics Research Center, Ehime University — Ice exhibits a wide variety of forms because of polarity of water molecules. More than fifteen forms including crystalline and amorphous phase have been reported so far. Among them ice VII and ice VIII have been known to have wide stability region, however, recent experimental and theoretical studies have suggested possible phase change and property change at around 10 to 15 GPa. The change has not yet sufficiently been explained. To obtain a clue for understanding the phase change, high pressure experiments were performed with deuterated and light water using DAC at room temperature. Raman spectroscopy showed that the peak width of OD vibrational mode became sharper at about 11 GPa with increasing pressure, and then it became broader again above the pressure. The squared vibrational frequency changed linearly with pressure, and the slope evidently change at about 14 GPa, indicating existence of phase change. In-situ X-ray diffractometry revealed splitting of diffraction line of cubic ice VII above 11GPa, which were indexed a tetragonal structure. The similar result was reported previously for light water. The tetragonal structure survived at least up to 60 GPa. All experimental results showed existence of phase change at around 11 GPa.

F1.00027 Freezing of liquid water under combined compression and electric fields, S.J.P. STAFFORD, S.N. BLAND, Imperial College, D.H. DOLAN, Sandia National Labs, D. EAKINS, Imperial College. INSTITUTE OF SHOCK PHYSICS COLLABORATION2, SANDIA NATIONAL LABS COLLABORATION3 — The melt curves of materials hold rich information concerning phase stability, coexistence, and other kinetics, typically studied through heating and cooling. Compression-induced solidification exposes new kinetics, yet it is a practical challenge due to adiabatic heating. Water has a large heat capacity and many solid phases, making it a good candidate for compression freezing. Optical transmission measurements and high-speed imaging have demonstrated that water can freeze on nanosecond time scales. Being highly polar, freezing in water is strongly influenced by electric fields at atmospheric pressure. However, the role of external electric fields in freezing has yet to be determined at high pressure. We present experimental and theoretical results from our attempts to transform liquid water into solid ice under rapid compression. To minimize heating, samples are quasi-isentropically compressed via multiple shock or ramp wave compression. An external electric field applied to the sample imparts local order to the system, influencing solidification onset and growth. Classical molecular dynamic simulations show significant ordering effects at V/nm field strength, well above the dielectric strength of water. We present work that to address this issue.

1 Freezing of liquid water under combined compression and electric fields 2 This PhD is sponsored through the ISP by the Atomic Weapons Establishment. (AWE) 3 Sandia National Labs is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the USDoE National Nuclear Security Administration under contract DE-AC04-94AL85000.

F1.00028 Raman scattering analysis of the structural phase transformations of III-V semiconductors induced by mechanical impact, PAULO PIZANI2, Universidade Federal de S˜ ao Carlos, Departamento de Física, RENATO JASINEVICIUS3, Universidade de S˜ ao Paulo, Escola de Engenharia de S˜ ao Carlos, NON HYDROSTATIC PRESSURES COLLABORATION — In the present work we report a Raman scattering study on the structural phase transitions of indium antimonide submitted to high non-hydrostatic pressure applied by mechanical impact, which induces several transformations, leading to very rich Raman spectra. We are able to observe the normal disordered zinc blende structure with a Raman spectrum displaying two broadened peaks at 180 and 190 cm\(^{-1}\), an amorphous phase with a Raman spectrum displaying only a broad band centered at about 175 cm\(^{-1}\), the optical band, that reflects the vibrational density of optical states, the wurtzite structure with Raman peaks at 145, 175 and 180 cm\(^{-1}\) and a completely new and intense Raman spectrum presenting fourteen lines. Similar results for GaAs and GaSb were also obtained.

1 Acknowledgements to FAPESP and CNpq funding agencies. 2CP 676, 13565-905 S˜ ao Carlos, SP 3Departamento de Engenharia Mecanica, CP 359, 13566-590 S˜ ao Carlos, SP

F1.00029 Resistivity and equations of state of warmed gallium melt in megabar pressure range, ANDREY GOLYSHEV, ALEXANDER MOLODETS, Institute of Problems of Chemical Physics RAS, Chernogolovka — The electrical conductivity of gallium melt was measured by shock channel up to 30-300 GPa. The semiempirical equation of state (EOS) are constructed in the shock pressure range 30-300 GPa. The EOS was used for reconstruction of thermodynamic history of the sample in the experiments and for the subsequent definition of volume-temperature dependence of gallium melt resistivity. It was shown that the resistivity is proportional to temperature and inversely to the square of characteristic temperature in the shock pressure range 30-80 GPa and temperatures 1000-2000 K. Thus the warmed high pressure gallium phase melt possesses metal conductivity.

F1.00030 Phase transition and electrical resistivities of PrBa\(_2\)Cu\(_4\)O\(_8\) under high pressures, YUH YAMADA, Dept. of Physics, Niigata Univ., AKIHIRO KOBAYASHI, NAOYA EGUCHI, Graduate School of Science and Technology, Niigata Univ., FUUMIHIO ISHIKAWA, Dept. of Physics, Niigata Univ., ATSUKO NAKAYAMA, AYAKO OHMURA, Center for Transdisciplinary Research, Niigata Univ., SATOSHI NAKANO, AKIYUKI MATSUSHITA, National Institute for Materials Science — PrBa\(_2\)Cu\(_4\)O\(_8\)(Pr124) does not exhibit superconductivity but its resistivity shows a metallic behavior below 170 K. This behavior is a sharp contrast to semiconducting one of PrBa\(_2\)Cu\(_3\)O\(_7\)+\(\delta\). This high pressure experiments were performed using Bridgman anvil type cell. The metallic region is found to be extended toward high temperatures with increasing pressure up to 5 GPa. The pressure dependence of the resistivity in room temperature is positive to 10 GPa while that is negative above 10 GPa. We have also studied the crystal structure of Pr124 means of the synchrotron radiation X-ray powder experiment under high pressure. High-pressure X-ray powder diffraction was performed at PF, BL-18C beamlines at room temperature using a diamond anvil cell (DAC). Up to 10 GPa, the diffraction patterns were fitted using the tetragonal Ammm symmetry model. The continuous change of lattice parameters as a function of pressure was observed. Furthermore, we confirmed the phase transition in Pr124 over 10 GPa. More detail results will be reported in this conference.

F1.00031 Transport properties of Pr Ba\(_2\)Cu\(_7\)O\(_{15-\delta}\) under high pressures, AKIYUKI MATSUSHITA, National Institute for Materials Science, SHUHEI YAMADA, Graduate School of Science and Technology, Niigata University, FUUMIHIO ISHIKAWA, Department of Physics, Niigata University, ATSUKO NAKAYAMA, AYAKO OHMURA, Center for Transdisciplinary Research, Niigata University, YUH YAMADA, Department of Physics, Niigata University — Pr Ba\(_2\)Cu\(_4\)O\(_7\)+\(\delta\) (Pr247) was found to exhibit superconductivity in 2004 by introducing oxygen deficiencies\[\text{Superconducting transition temperature (Tc) varies from zero to about 20 K depending on the oxygen deficiency }\delta.\] This high Tc cuprate consists of three structural units, i.e., CuO\(_2\) planes, CuO single chain and CuO\(_2\) double chains. The CuO\(_2\) planes are insulating in this compound and therefore, the superconductivity is believed to occur in the CuO\(_2\) double chains. Interestingly, the electrical resistivity was found to show T\(^2\) dependence at low temperatures under high magnetic fields. This temperature dependence is known as the characteristic property of Tomonaga-Luttinger liquid and suggests a possibility that the CuO\(_2\) double chains have one-dimensional property. In this study we report the pressure dependence of the transport properties for Pr247 with various oxygen deficiency \(\delta\)’s.

The effect of pressure on reaction rates is traditionally expressed in terms of logarithmic pressure derivatives, known as activation volumes. According to TST, identification of the TS difficult using traditional molecular dynamics (MD) techniques. We propose to identify TS structures using their volumetric properties.

In this paper, the high-pressure phase diagram of the binary system has been investigated by examining the x-ray diffraction patterns of the polycrystalline data show the well known antiferromagnetic-to-paramagnetic transformation near 174 K. The pressure coefficient of resistance at room temperature is somewhat lower than found by Bridgman, probably reflecting a higher purity of the material. The pressure coefficient is observed to decrease with increasing temperature.

Recently, in the mixture of oxygen and nitrogen molecules, the appearance of a new solid phase, which does not occur for either pure component, has been reported under high pressure. We consider that the magnetic interaction of oxygen molecules would play a main role of the formation of the phase. In this paper, the high-pressure phase diagram of the binary system has been investigated by examining the x-ray diffraction patterns of the polycrystalline or powder samples. The solid phase was stable in a rather wide pressure and concentration range than previous report. From the Reitveld refinement the structure of the phase was identified to be a hexagonal structure with seven molecules in the unit cell. The results of x-ray diffraction, Raman scattering and magnetization measurements have suggested a magnetic order of oxygen molecules on the Kagome-lattice.
F1.00038 Elastic properties of methane-propane mixed gas hydrate under high pressure. SHINYA MIWA, MASAKI KANOU, TETSUJI KUME, SHIGEO SASAKI, Department of Materials Science and Technology, Gifu University — Methane hydrate (MH) is widely observed in Earth's environment such as permafrost and deep sea floors. At low temperature and low pressure conditions, pure MH crystallizes a cubic structure I (s) which consists of hydrogen-bonded two small and six medium water cages which enclathrate methane molecules as guests. However, actual MH in deep sea deposits contains not only methane molecules but also ethane and propane molecules. Therefore, the estimation of elastic properties and mechanical stability for both sI and structure II (sII) are required for the safe extraction of methane gas from the deep sea floors. The purpose of this study is to determine the elastic properties of methane-propane mixed gas hydrate (MHP) with sII by applying the high-pressure Brillouin spectroscopy to a single crystal of MHP-sII grown in a diamond anvil cell. The obtained elastic constant C11 of MHP-sII showing independent of pressure is obviously different from that of pure MH-sI. On the other hand, the C12 and C44 are similar to MH-sI. The present results suggest that a variety of gas hydrates have the individual elastic properties and stability depending on the gas hydrate structures.

F1.0039 Energetic Lnacthiide Complexes: Coordination Chemistry and Explosives Applications. VIRGINIA MANNER, BEAU BARKER, ERIC SANDERS, KENNETH LAINTZ, BRIAN SCOTT, DANIEL PRESTON, MARY SANDSTROM, BETTINA REARDON, Los Alamos National Laboratory. Metals are generally added to organic molecular explosives in a heterogeneous composite to improve overall heat and energy release. In order to avoid creating a mixture that can vary in homogeneity, energetic organic molecules can be directly bonded to high molecular weight metals, forming a single metal complex with Angstrom-scale separation between the metal and the explosive. To probe the relationship between the structural properties of metal complexes and explosive performance, a new series of energetic lanthanide complexes has been prepared using energetic ligands such as NTO (5-nitro-2,4-dihydro-1,2,4-triazole-3-one). These are the first examples of lanthanide NTO complexes where no water is coordinated to the metal, demonstrating novel control of the coordination environment. The complexes have been characterized by X-ray crystallography, NMR and IR spectroscopies, photoluminescence, and sensitivity testing. The structural and energetic properties are discussed in the context of enhanced blast effects and detection. CHEETAH calculations have been performed to fine-tune physical properties, creating a systematic method for producing explosives with “tailor made” characteristics. These new complexes will be benchmarks for further study in the field of metalized high explosives.

F1.0040 New high-pressure perovskite-like phases ACuV4O12 (A-Sm, Gd, Tb, Dy, Er and Tm): synthesis and electrical properties. IRINA USTINOVNA, NINA MELNIKOVA, UnFU, NADEZHDA KADYROVA, ISSC UB RAS, ALEXEY BABUSHKIN, UnFU, YURIY ZAYNULIN, ISSC UB RAS — The aim of this work was to investigate the effect of high pressures on the electrical properties of the new high-pressure perovskite-like phases ACuV4O12 (A-Sm, Gd, Tb, Dy, Er and Tm). The X-ray and microstructural studies of the synthesized by barothermal compression compounds were carried out. The electrical properties of the compounds were studied in the wide ranges of frequencies of the electric field, temperatures and pressures.

3 This work was supported in part by the Russian Foundation for Basic Research, project 12-02-31607. Also the research was carried out in terms of Ural Federal University development program with the financial support of young scientists.

F1.0041 Single walled carbon nanotubes at ultra-high pressure/stress. MAXIME NOEL, MATTIAS MASES, Division of Physics, Department of Engineering Sciences and Mathematics, Luleå University of Technology, SE-97187, Luleå, Sweden, ALEXANDER V. SOLDATOV. Division of Physics, Department of Engineering Sciences and Mathematics, LuleåUniversity of Technology, SE-97187, Luleå, Sweden — We report on the first study of single walled nanotubes (SWCNTs) synthesized by HiPCO method under pressure/stress up to 70 GPa aimed at probing structural stability of small diameter SWCNTs and synthesis of new nanostructured carbon phases. Firstly, the material has been exposed to 25 GPa. Raman spectra of the recovered of material exhibited extremely high defect density and evident recovery of the radial breathing mode (RBM) band with some intensity profile alteration. Secondly, the material was pressurized subsequently to 70 GPa followed by a relatively fast pressure release. Raman characterization provides indications of a transformation of the material to a new structural state as the result of the second pressure cycle. We discuss the structural evolution of the system en-route the final structure which is presumably comprised of deformed graphene nanoribbons and/or polymerized CNTs in addition to the smallest diameter SWCNTs which survived ultra-high pressure/stress.

2 Other affiliation: Department of Physics, Harvard University, Cambridge, MA-02138, USA / Corresponding author: Alexander.Soldatov@ltu.se

F1.0042 High-pressure high-temperature behavior of polymer derived amorphous B-C-N1, S. BHAT, S. LAUTERBACH, D. DZIVENKO, H. KLEEPE, R. RIEDEL, TU Darmstadt, Germany, C. LATHE, GFZ Potsdam, Germany, L. BAYARTJARGAL, B. WINKLER, Goethe University Frankfurt, Germany, M. SCHWARZ, E. KROKE, TU Bergakademie Freiberg, Germany — Dense diamond-like BCN compounds are of interest due to their extreme hardness and predicted exceptional thermal and chemical stability superior to diamond and c-BN. Here, we report on high-pressure high-temperature (HP-HT) behavior of amorphous BC$_N$ and BC$_N$ — potential precursors for HP-HT synthesis of diamond-like BCN. Prepared via hydroboration reaction of piperazine borane and pyridine borane, respectively, amorphous BC$_2$N and BC$_2$N are characterized by well-mixed B-N, C-C and C-N bonds, confirmed by XPS analysis. These BCN compositions were subjected to pressures between 5-24 GPa and temperatures up to 2000°C using multi anvil press, torroid press and laser-heated diamond anvil cell (LH-DAC). In- and ex-situ X-ray diffraction reveals decomposition of BC$_N$ to graphite and h-BN between 5 to 12 GPa above 700°C, in contrast to BC$_2$N which remains amorphous up to 1600°C. Examination of the recovered LH-DAC samples using HR-TEM, EELS and EDS, indicates a tendency of BC$_N$ to transform into a mixture of c-BN (micron size) and nanocrystalline diamond between 20-24 GPa and 1500-2000°C.

1Financially supported by the DFG within SPP 1236.


F1.0043 Diamond Anvils Using Nano-polycrystalline Diamonds for the High-pressure Generation. YUKI NAKAMOTO, MASAFUMI SAKATA, Osaka University, HITOSHI SUMIYA, Sumitomo Electric Industries, KENJI OHTA, TAKAHIRO MATSUOKA, KATSUYA SHIMIZU, Osaka University, TETSUO IRIFUNE, Ehime University, YASUO OHISHI, JASRI/SPring-8, CENTER FOR QUANTUM SCIENCE AND TECHNOLOGY UNDER EXTREME CONDITIONS COLLABORATION, ELECTRONICS & MATERIALS R&D LAB, COLLABORATION, GEO-DYNAMICS RESEARCH CENTER COLLABORATION, JAPAN SYNCHROTRON RADIATION RESEARCH INSTITUTE COLLABORATION — Diamond-anvil (DAC) technique with natural single crystal diamonds (SDD) as anvils is widely used for high-pressure experiments. High-purity nano-polycrystalline diamond (NPD) consists of very fine diamond grains of several 10s of nanometer oriented in random directions, and has extremely high hardness comparable to or even harder than SDD[1]. The NPD has neither the cleavage feature nor the anisotropy of hardness peculiar to SCD, and has high fracture toughness[2]. We have examined some high pressure generation pilot tests using the diamond anvils prepared from the NPD [3][4][5]. The pressures were determined by the EOS of Pt. A powder X-ray diffraction experiment of Pt was carried out using a synchrotron radiation on BL10XU at SPring-8. Some high-pressure generating tests were performed using diamond anvils of various shapes prepared from NPDs. The achievable pressure value of an NPD anvil with a culet size of more than 0.3 mm is about 1.5 to 2 times higher than that of SCD anvils, indicating that NPD anvils have considerable potential for large-volume diamond anvils with large culet sizes. Furthermore, we consider about beveled culet and lateral supported bottom shape on NPD anvil. It was found that the generated pressure is increased 2.5 times higher than the SCD anvil with normal anvil shape. [1] T. Irifune et al., Nature, 421, 599(2003). [2] H. Sumiya and T. Irifune, J. Mater. Res., 22, 2345(2007). [3] Y. Nakamoto et al., Jpn. J. Appl. Phys. 46, L640 (2007). [4] Y. Nakamoto et al., Rev. Sci. Inst. 82, 066104 (2011).
Profiles from the gauges indicate that wave instabilities grow as the overdriven detonation wave settles down following the shock-to-detonation transition. For example, little change in overtake time occurs in 80 wt%/20 wt% NM/methanol when compared with neat NM. Furthermore, the shock wave is a function of shock input condition for mixture concentrations from 100% NM to 50 wt%/50 wt% NM/methanol. Desensitization with dilution is less than expected. BAUM, STEVE SHEFFIELD, LEE GIBSON, Los Alamos National Lab — The dilution of liquid explosives has multiple effects on detonation properties including lowering of the Chapman-Jouguet detonation pressure, and 3) slowing of the steady detonation velocity (Koldunov, et al. Comb. Expl. Shock Waves). Here, we present the results of a series of gas gun-driven plate-impact experiments to study the shock-to-detonation transition in NM/methanol mixtures. Embedded electromagnetic gauges were used to obtain in situ particle velocity wave profiles at multiple Lagrangian positions in the initiating explosive mixture. From these experiments, we conclude that the shock-to-detonation transition is triggered by: 1) a continual increase in the critical diameter, 2) lowering of the Chapman-Jouguet detonation pressure, and 3) slowing of the steady detonation velocity (Koldunov, et al. Comb. Expl. Shock Waves). Here, we present the results of a series of gas gun-driven plate-impact experiments to study the shock-to-detonation transition in NM/methanol mixtures. Embedded electromagnetic gauges were used to obtain in situ particle velocity wave profiles at multiple Lagrangian positions in the initiating explosive mixture. From the wave profiles obtained in each experiment, an unreacted Hugoniot locus, the initiation mechanism, and the overtake-time-to-detonation were obtained as a function of shock input condition for mixture concentrations from 100% NM to 50 wt%/50 wt% NM/methanol. Desensitization with dilution is less than expected. Furthermore, the shock wave profiles from the gauges indicate that wave instabilities grow in as the overdriven detonation wave settles down following the shock-to-detonation transition.
F1.00050 Using laser-driven flyer plates to study the shock initiation of nanoenergetic materials, WILLIAM SHAW, DANA DŁOTT, University of Illinois at Urbana — A tabletop system has been developed to launch aluminum laser-driven flyer plates at speeds up to 4 km/s. The flyer plates are used to initiate a variety of nanoenergetic materials including aluminum/iron oxide particles produced by arrested ball milling, and multi-layer nano-thermites produced by sputtering. The initiation process is probed by a variety of high-speed diagnostics including time-resolved emission spectroscopy. Impact velocity initiation thresholds for different thickness flyer plates, producing different duration shocks, were determined. The durations of the emission bursts and the effects of nanostructure and microstructure on these bursts were used to investigate the fundamental mechanisms of impact initiation.

F1.00051 Impact Initiated Combustion of Aluminum Exposed to Mechanical Pre-Activation1, JENNIFER BREIDENICH, NAРЕSH THADHANI, Georgia Institute of Technology — The impact initiation of as-received and mechanically activated aluminum powder compacts is investigated using uniaxial stress rod-on-anvil impact experiments. The compacts reveal light emission due to combustion reaction at velocities greater than 320m/s. Mechanical pre-activation, such as that achieved via high-energy ball milling (HEBM) or high strain machining, strain hardens the starting materials, affecting their combustion initiation behavior. The starting materials are characterized by their lattice strain, hardness, and quasi-static compaction behavior. High speed imaging reveals that the “threshold” velocity (minimum velocity necessary for reaction initiation) changes as function of the mechanical pre-activation. Meso-scale simulations performed in CTH are used to correlate the effects of material properties within the powder compact with the crush up, deformation, and reaction behavior.

1Research funding provided by DTRA Grant No. HDTRA1-10-1-0038

F1.00052 Pressure-induced transformations of bis(tetrazolyl)amine and cyanuric triazide probed by vibrational spectroscopy and X-ray diffraction, YANG SONG, LIANG ZHOU, ERICA TILL, University of Western Ontario, ANGJUANG HU, Defense Research and Development Canada — As promising high energetic materials, bis(tetrazolyl)amine (BTA) and cyanuric triazide (CTA) have been studied extensively due to their high nitrogen content. Here we report the first in situ high-pressure study of BTA and CTA using vibrational spectroscopy and synchrotron X-ray diffraction. A reversible phase transformation of BTA was observed in the compression-decompression cycle. For CTA, we observed an interesting phase transformation as evidenced by the color change of the sample as well as the change in the Raman profile and X-Ray diffraction patterns. The transformations of BTA and CTA provide more understanding of the high-pressure behavior of nitrogen-rich materials and guidance for the further developments of energetic materials.

F1.00053 ABSTRACT WITHDRAWN

F1.00054 Tilt Correction of High Explosive Test Data with Examples, LARRY HILL, ELIZABETH FRANCOIS, JOHN MORRIS, Los Alamos National Laboratory — Many high-explosive experiments view a nominally-axially-symmetric detonation wave breaking through a charge surface. Emerging waves virtually always exhibit a degree of tilt, which one generally wants to excise from the data whilst quantifying its direction and magnitude. In some cases, such as front-curvature rate sticks and Onionskin (OS)-type tests, the diagnostic is a single-slit streak camera (1D correction). In other cases, such as a Plane-Wave Lens characterization test or a Furball test, multiple slits or fibers provide sparse data over a surface (2D correction). We demonstrate both 1D and 2D corrections, the latter of which is the more challenging. In 2D, we represent the breakout time as the sum of a symmetric component and an asymmetric component (a tilted plane). The two tilt angle components are found that minimize the data scatter associated with the symmetric component. The most compelling example is the Furball test, an OS-variant for which the breakout time over the hemispherical observation surface is measured at many points using optical fibers. Unlike the OS test that looks in one (random) direction, we are able to construct OS-type data in the direction of maximum tilt, even though there are generally no fibers at that direction.

F1.00055 Shock initiation of the TATB-based explosive PBX 9502 cooled to 77 Kelvin, B.C. HOLLOWELL, R.L. GUSTAVSEN, D.M. DATTELBAUM, B.D. BARTRAM, Los Alamos National Laboratory — Recently we reported on shock initiation of PBX 9502 (95 wt. % tri-amino-trinitro-benzene, 5 wt. % Kel-F800 binder) cooled to -55°C or 218K (J. Appl. Phys., 112, 74909 (2012)). Shock waves were generated by gas-gun driven plate impacts and reactive flow in the cooled PBX 9502 was measured with embedded electromagnetic gauges. Here we describe methods to cool the explosive below -55°C, down to liquid nitrogen temperature of -196°C or 77K. We start cooling by flowing chilled nitrogen (N2) gas through channels in a sample mounting plate and a copper tubing coil. Temperature in the sample is monitored using type-E thermocouples; samples are cooled at ≈1-2°C/min. After minimum temperature is reached using N2 gas, we flow liquid nitrogen (LN2) through the channels. Minimum temperatures of 77K were reached. Preliminary results show continued reductions in temperature cause continued reductions in shock sensitivity. Reducing the temperature below -55°C further reduces the sensitivity. Wave profiles were also obtained during the shock-to-detonation transition and will be presented.

F1.00056 Explosive acceleration of plates using nonconventional explosives heavily loaded with inert and reactive materials, JASON LOISEAU, OREN PETEL, JUSTIN HUNEAULT, MATTHEW SERGE, DAVID FROST, ANDREW HIGGINS, McGill University, Mechanical Engineering Dept., 817 Sherbrooke St. W., Montreal, Quebec, H3A 2K6, Canada — The detonation behavior of high explosives containing dispersed quantities or packed beds of dense additives has been previously investigated with the observation that such systems depart from the “gamma law” behavior typical of homogeneous explosives and the temperature and the shock energy remain strongly coupled to the density of the reactive elements. However, the influence of the non-ideal detonation behavior on the divergent speed of plates has been less rigorously studied and existing literature suggests that the effect of dense additives cannot be explained solely through the straightforward application of the Gurney method with energy and density averaging. In the current study, the acceleration history and terminal velocity of aluminum flyers launched by packed beds of granular material saturated by amine-sensitized nitromethane is reported. Two experimental configurations are used to study acceleration either by a purely grazing detonation in a finite thickness slab of explosive or by a normal detonation from an effectively infinite thickness of explosive. Flyer acceleration and velocity is measured via Photonic Doppler Velocimetry. Packed beds of plastic, aluminum, glass, iron, and bismuth are considered and the data is compared to Gurney velocity predictions.

F1.00057 Small-Scale Tunnel Tests for Blast Performance, JOSHUA FELTS, RICHARD LEE, NSWC Indian Head — The data reported here provides a validation of a small-scale tunnel test as a tool to guide the optimization of new explosives for blast performance in tunnels. The small-scale arrangement consisted of a 2-g booster and 10-g sample mounted at the closed end of a 127-mm diameter by 4.6-m long steel tube with pressure transducers along its length. The three performance characteristics considered were peak pressure, initial energy release, and impulse. The relative performance from six explosives was compared to that from a 1.16-m diameter by 30-m long tunnel that used 2.27-kg samples. The peak pressure and impulse vs. distance did not scale between the small and larger scale tests but the relative ranking was preserved. The initial energy release was determined from a one-dimensional point-source analysis, which tracked with peak pressure vs. distance results but not with impulse suggesting additional energy released further down the tunnel for some explosives. This test is a viable tool for optimizing compositional variations for blast performance in target scenarios of similar form factor.
**F1.00058 Small-Scale Chamber Test for Internal Blast Performance**, RICHARD LEE, JOSHUA FELTS, NSWC Indian Head — The data reported here provides a validation of the use of a small-scale internal-blast test to predict the energy release of explosives in larger scale. The small-scale arrangement consisted of a 2-g booster and 10-g sample mounted in a holder attached at one end of a closed chamber. The internal volume of the chamber was 89 liters not including the charge holder. The design of the charge holder served two purposes. One was to provide confinement around the charge to avoid degradation of performance from explosives with critical diameters larger than that of the sample. The second was to provide a separate space from that of the chamber that retained the fragments from the confinement to minimize the absorption of heat from the products. The energy release was determined from measurements of the peak quasi-static overpressure and the ideal gas law. The results from six different explosives were compared to larger scale tests involving a bombproof chamber (180,000 liters) with bare charges between 1 and 16 kg. The energy release between small and large scale compared favorably with regard to relative ranking of each explosive. The energy release measured in the small chamber was lower than the large chamber analogs, possibly due to heat losses to the holder. Despite these differences, the small-scale chamber test appears to provide a ranking of explosives based on their energy release that correlates with larger scale tests. Hence, this test is a viable tool for optimizing compositional variations for internal blast performance in target scenarios of similar form factor.

**F1.00059 High and Low Velocity Detonation in a HighlyInsensitive Explosive**, HAROLD SANDUSKY, HEATHER HAYDEN, NSWC Indian Head — TBD

**F1.00060 Modified Reaction Detection Methods on the Drop Weight Impact Machine**, DANIEL PRESTON, GEOFFREY BROWN, JOSEPH KOBY, LANL — High explosives small-scale sensitivity testing has been a hallmark of safety screening since WWII. Sensitivity testing was once as crude as using the end of a broom stick to scrape explosives on the floor, looking, listening, and smelling for signs of reaction. Since then, a wide variety of testing apparatus have been developed to explore the effects of different stimuli on explosives. In concert with the development of the machines themselves the reaction detection methods have also evolved. Some modern detection devices include sound level meters, high speed cameras, and light detection sensors to name a few. For this paper, the viability of new and modified reaction detection methods employed on the LANL Explosives Research Laboratory (ERL) Type 12 Drop Weight Impact Machine is explored. A large bandwidth microphone and a series of strain gauges were installed on the machine and, with an oscilloscope, were able to capture the acoustic and mechanical wave forms during an impact event. These data were then used as a metric for developing reaction criteria for explosives on drop weight impact.

**F1.00061 Reactivity of Ti-B, Cr-S, and Mn-S powder systems during explosively-driven collapse**, MATTHEW SERGE, ATEFEH NABAVI, McGill University, PO-HSUN CHIU, University of California, San Diego, ANDREW HIGGINS, McGill University, VITALI NESTERENKO, University of California, San Diego — Metal-metal and metal-sulfur reactive powder mixtures have been previously tested for initiation of reaction via planar, normal-shock loading. In addition to reacting under shock, such powder mixtures may undergo exothermic reaction under other types of mechanical loading. The thick-walled cylinder (TWVC) technique was performed on samples of Ti-B (1:2 molar ratio), Cr-S (1:1.5:1 molar ratio), and Mn-S (1:1 molar ratio). These experiments were performed to determine the effect of large shear strains exerted on reactive metal powder mixtures and to establish the relative effectiveness of shear loading in comparison to shock loading in initiating reaction. Recovered samples were analyzed via SEM and XRD to determine the degree of reaction.

1Funding was provided in part by ONR MURI N00014-07-1-0740 (Program Officer Dr. Clifford Bedford)

**F1.00062 The effect of hydrostatic vs. shock pressure treatment on plant seeds**, ADRIAN MUSTEY, JAMES LEIGHS, GARETH APPLEBY-THOMAS, DAVID WOOD, Cranfield University, RACHAEL HAZAEL, PAUL MCMILLAN, University College London, PAUL HAIZEL, University of New South Wales — The hydrostatic pressure and shock response of plant seeds have both been previously investigated (primarily driven by an interest in reducing bacterial contamination of crops and the theory of panspermia respectively). However, comparisons have not previously been made between these two methods of applying pressure to plant seeds. Here such a comparison has been undertaken based on the premise that any correlations in such data may provide a route to inform understanding of damage mechanisms in the seeds under test. In this work two varieties of plant seeds were subjected to hydrostatic pressure via a non-end-loaded piston cylinder set-up and shock compression via employment of a 50-mm bore, single stage gas gun using the flyer-plate technique. Results from germination tests of recovered seed samples have been compared and contrasted, and initial conclusions made regarding causes of trends in the resultant data set.

**F1.00063 Development of Experimental Tissue Models for Blast Injury**, BENJAMIN BUTLER, Department of Physics, University of Cambridge, CHIARA BO, Institute of Shock Physics, Department of Physics, Imperial College London, ALUN WILLIAMS, Department of Veterinary Medicine, University of Cambridge, ANDY JARDINE, KATHERINE BROWN, Department of Physics, University of Cambridge — There is a pressing need to better understand the relationship between the intensity of a blast wave and the clinical consequences for victims of an explosion. In order to quantitatively study how these factors correlate with one another, blast injury tissue models are being developed. Sections of larynx, trachea and pulmonary tissue were excised from a recently sacrificed pig and maintained on ice prior to testing. The samples were subjected to strain rates of between 0.001 s⁻¹ and 1000 s⁻¹ in the laboratory by using a Split Hopkinson Pressure Bar and quasi-static testing apparatus. During high strain rate testing, samples were housed in a polycarbonate chamber which permitted experimentation on tissue held in fluid. Data were analysed using 1, 2 and 3 wave analysis software in Matlab to yield information about the material properties of both undamaged and damaged tissues. In addition, macroscopic changes in tissue organization were also visualized using histopathological techniques. This work is being extended to cellular and animal models to derive more detailed information about the underlying molecular changes relating to blast-induced damage and repair.

1The Royal British Legion Centre for Blast Injury Studies

**F1.00064 Ultrafine particle generation by high-velocity impact of metal projectiles**, GIANLUCA STABILE, PAOLO VIGO, ANDREW RUGGIERO, ALDO RUSSI, GIORGIO BUONANNO, University of Cassino and Southern Lazio — In the present work, size distributions and total concentrations of ultrafine particles generated during high velocity impacts of metals are shown in order to estimate the possible exposure of survival personnel to ultrafine metallic particles in the event of kinetic energy penetrator impact. Taylor cylinder impact tests were designed and performed using a light gas-gun facility investigating both high purity copper and aluminium cylinders impacting against a steel anvil in impact chamber. Moreover, in order to deepen the possible particle formation mechanisms, ballistic impact tests without metal-on-metal sliding contacts were also performed. In particular, symmetrical Taylor impacts of copper cylinders tests (rod-on-rod tests) were designed. High-resolution time measurements of particle distributions and total concentrations were performed through Fast Mobility Particle Sizer spectrometer and Condensation Particle Counters. Particle number emission factors were also evaluated. High particle generation in the ultrafine range were detected in classic Taylor cylinder impact tests: particle number distributions with a mode of 10 nm were detected. Moreover, number emission factors comparable to the ones typical of combustion phenomena were recognized.
The results obtained to date indicate that in spite of the wave reflections and reverberations within the coupon, the particle-coupon interface response can be understood as friction. The spatial and temporal average stresses and strains at the particle-coupon interface are compared with the in-situ shock response of the particle. The particle mounted with a 1.8 micron thick epoxy coupon impacted by a 60 micron aluminum ball at 500 m/s. The impact is considered for the particle alone and the coupon together. The ongoing work is an attempt to address a yet unresolved question; how a complex non-uniaxial thermomechanical shock response at the mesoscale, which may be a precursor to more complex phenomena, correlates to the average continuum uniaxial shock response. The objective of this work is to gain insight into how the complex responses at the meso/sub-mesoscale manifest to quantities that could be experimentally measured without perturbing the material. The simulations consider a 60 micron spherical sand particle mounted with a 1.8 micron thick epoxy coupon impacted by a 60 micron aluminum ball at 500 m/s. The impact is considered for the particle alone (direct impact) as well as embedded within an assembly of 100 particles of the same size (indirect impact). Particle contact is modeled with and without friction. The spatial and temporal average stresses and strains at the particle-coupon interface are compared with the in-situ shock response of the particle. The results obtained to date indicate that in spite of the wave reflections and reverberations within the coupon, the particle-coupon interface response can be statistically correlated to the in-situ shock response.

This work is supported in part by DTRA Grant HDTRA-12-1-0052 and AFOSR Grant FA 9550-12-1-0128.

Mechanoluminescence of nylon under high velocity impact. NICOLA BONORA, ANDREW RUGGIERO, University of Cassino and Southern Lazio, GIANLUCA IANNITTI, Techdyn Engineering, CARMINE ABBATE, FRANCESCO IANNUZZO, GIOVANNI BUSATTO, University of Cassino and Southern Lazio — This work presents an experiment involving the generation of a mechanical shock due to the impact of a large aluminum sphere on a nylon coupon. The impact is considered for the particle alone and the coupon together. The ongoing work is an attempt to address a yet unresolved question; how a complex non-uniaxial thermomechanical shock response at the mesoscale, which may be a precursor to more complex phenomena, correlates to the average continuum uniaxial shock response. The objective of this work is to gain insight into how the complex responses at the meso/sub-mesoscale manifest to quantities that could be experimentally measured without perturbing the material. The simulations consider a 60 micron spherical sand particle mounted with a 1.8 micron thick epoxy coupon impacted by a 60 micron aluminum ball at 500 m/s. The impact is considered for the particle alone (direct impact) as well as embedded within an assembly of 100 particles of the same size (indirect impact). Particle contact is modeled with and without friction. The spatial and temporal average stresses and strains at the particle-coupon interface are compared with the in-situ shock response of the particle. The results obtained to date indicate that in spite of the wave reflections and reverberations within the coupon, the particle-coupon interface response can be statistically correlated to the in-situ shock response.

The effect of fibre orientation on a TWCP composite. NICHOLAS BARNES, AWE, DAVID WOOD, GARETH APPLEBY-THOMAS, JAMES LEIGHS, ANDREW ROBERTS, Cranfield University, PAUL HAZELL, The University of New South Wales — Multiple authors have shown that orientation can greatly affect the shock profiles seen in composites. Carbon fibre composites are employed in multiple sectors, with their use in the aerospace industry becoming more prevalent. An angle of 20° between strength and ablation. Using a single stage gas gun with manganin pressure gauges the shock response of both a 90° and 45° layup TWCP composite were investigated up to a particle velocity of c.a. 1 mm/s. In both the U3-ut, and pressure-volume plane. Comparisons in terms of shock propagation were also made with previously investigated TWCP orientations of 0° and 20° as well as other carbon fibre based composites from the literature. This allowed a detailed interrogation of the effects of weave orientation in this important TWCP composite to be made.

High strain rate fracture behavior of fused silica. ANDREW RUGGIERO, University of Cassino and Southern Lazio, GIANLUCA IANNITTI, Techdyn Engineering, GABRIEL TESTA, University of Cassino and Southern Lazio, JEROME LIMIDO, JEAN LUC LACOME, LARS OLOVSSON, IMPETUS-APEA, MARIO FERRARO, MBDA Italia, NICOLA BONORA, University of Cassino and Southern Lazio — Fusion silica is a high purity synthetic amorphous silicon dioxide characterized by low thermal expansion coefficient, excellent optical qualities and exceptional transmittance over a wide spectral range. Because of its wide use in the military industry as window material, it may be subjected to high-energy ballistic impacts. Under such dynamic conditions, post-impact response of the ceramic as well as the strain rate related effects become significant and should be accounted for in the constitutive modeling. In this study, the procedure for constitutive model validation and model parameters identification, is presented. Taylor impact tests and drop weight tests were designed and performed at different impact velocities, from 1 to 100 m/s, and strain rates, from 100 up to 104 s⁻¹. Numerical simulation of both tests was performed with IMPETUS-FEA, a general non-linear finite element software which offers Nurbs finite element technology for the simulation of large deformation and fracture in materials. Model parameters were identified by optimization using multiple validation metrics. The validity of the parameters set determined with the proposed procedure was verified comparing numerical predictions and experimental results for an independent designed test consisting in a fused silica tile impacted at prescribed velocity by a steel sphere.

This work presents an experiment involving the generation of a mechanical shock due to the impact of a large aluminum sphere on a nylon coupon. The impact is considered for the particle alone and the coupon together. The ongoing work is an attempt to address a yet unresolved question; how a complex non-uniaxial thermomechanical shock response at the mesoscale, which may be a precursor to more complex phenomena, correlates to the average continuum uniaxial shock response. The objective of this work is to gain insight into how the complex responses at the meso/sub-mesoscale manifest to quantities that could be experimentally measured without perturbing the material. The simulations consider a 60 micron spherical sand particle mounted with a 1.8 micron thick epoxy coupon impacted by a 60 micron aluminum ball at 500 m/s. The impact is considered for the particle alone (direct impact) as well as embedded within an assembly of 100 particles of the same size (indirect impact). Particle contact is modeled with and without friction. The spatial and temporal average stresses and strains at the particle-coupon interface are compared with the in-situ shock response of the particle. The results obtained to date indicate that in spite of the wave reflections and reverberations within the coupon, the particle-coupon interface response can be statistically correlated to the in-situ shock response.

F1.00065 Femtosecond laser-driven shock-induced lattice defects in iron. TOMOKI MATSUDA, Osaka University, TOMOKAZU SANDE, Osaka University & JST-CREST, KAZUTO ARAKAWA, Shimane University & JST-CREST, AKIO HIROSE, Osaka University — We found high-density lattice defects such as microbands and twins in the femtosecond laser-driven shocked-pure iron. We used two kinds of femtosecond laser pulses of 1.5 × 10¹⁴ W/cm² and 9.8 × 10¹⁴ W/cm² to drive a weaker shock wave for multiple shots and a stronger one for single shot, respectively. TEM images and EBSE analysis showed that the former created microbands organized by high-density dislocations and the latter twins. We suggest that microbands are formed by pile-up of dislocations which is promoted by their interactions in multiple shots and that the twinning occurs owing to the high-strain rate which is strong enough to induce high-pressure phase. The process of lattice defects formation will be addressed in the presentation.

F1.00066 Correlating Computationally Derived Particle Surface Stress-Strain States to Mesoscale Shock Response. DAVID SCRIPKA, SUNIL DWIVEDI, NARESH THADHANI, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332 — The results of 2D and 3D FE simulations are presented, correlating the in-situ mesoscale shock response at the particle level to their surface observable stresses-strains for possible future experimental measurements. The ongoing work is an attempt to address a yet unresolved question; how a complex non-uniaxial thermomechanical shock response at the mesoscale, which may be a precursor to more complex phenomena, correlates to the average continuum uniaxial shock response. The objective of this work is to gain insight into how the complex responses at the meso/sub-mesoscale manifest to quantities that could be experimentally measured without perturbing the material. The simulations consider a 60 micron spherical sand particle mounted with a 1.8 micron thick epoxy coupon impacted by a 60 micron aluminum ball at 500 m/s. The impact is considered for the particle alone (direct impact) as well as embedded within an assembly of 100 particles of the same size (indirect impact). Particle contact is modeled with and without friction. The spatial and temporal average stresses and strains at the particle-coupon interface are compared with the in-situ shock response of the particle. The results obtained to date indicate that in spite of the wave reflections and reverberations within the coupon, the particle-coupon interface response can be statistically correlated to the in-situ shock response.

Mechanoluminescence of nylon under high velocity impact. NICOLA BONORA, ANDREW RUGGIERO, University of Cassino and Southern Lazio, GIANLUCA IANNITTI, Techdyn Engineering, CARMINE ABBATE, FRANCESCO IANNUZZO, GIOVANNI BUSATTO, University of Cassino and Southern Lazio — This work presents an experiment involving the generation of a mechanical shock due to the impact of a large aluminum sphere on a nylon coupon. The impact is considered for the particle alone and the coupon together. The ongoing work is an attempt to address a yet unresolved question; how a complex non-uniaxial thermomechanical shock response at the mesoscale, which may be a precursor to more complex phenomena, correlates to the average continuum uniaxial shock response. The objective of this work is to gain insight into how the complex responses at the meso/sub-mesoscale manifest to quantities that could be experimentally measured without perturbing the material. The simulations consider a 60 micron spherical sand particle mounted with a 1.8 micron thick epoxy coupon impacted by a 60 micron aluminum ball at 500 m/s. The impact is considered for the particle alone (direct impact) as well as embedded within an assembly of 100 particles of the same size (indirect impact). Particle contact is modeled with and without friction. The spatial and temporal average stresses and strains at the particle-coupon interface are compared with the in-situ shock response of the particle. The results obtained to date indicate that in spite of the wave reflections and reverberations within the coupon, the particle-coupon interface response can be statistically correlated to the in-situ shock response.

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F1.00071 Deformation and Fracture Behavior of Steel Projectiles Impact AD95 Ceramic Targets-Experimental Investigation1. GANG WEI, WEI ZHANG, Harbin Institute of Technology — The deformation and fracture behavior of steel projectile impacting ceramic target is an interesting investigation topic. The deformation and failure behavior of projectile and target was investigated experimentally in the normal impact by different velocities. Lab-scale ballistic tests of AD95 ceramic targets with 20 mm thickness against two different hardness 38CrSi steel projectiles with 7.62 mm diameter have been conducted at a range of velocities from 100 to 1000 m/s. Experimental results show that, with the impact velocity increasing, for the soft projectiles, the deformation and fracture modes were mushrooming, shear cracking, petalling and fragmentation(with large fragments and less number), respectively, for the hard projectiles there are three deformation and fracture modes: mushrooming, shearing cracking and fragmentation(with small fragments and large number). All projectiles were rebound after impact. But, with the velocity change, the target failure modes have changed. At low velocity, only radial cracks were found; then circumferential cracks appeared with the increasing velocity; the ceramic cone occurred when the velocity reached 400 m/s above, and manifested in two forms: front surface intact at lower velocity and perforated at higher velocity. The higher velocity, the fragment size is smaller and more uniform distribution. The difference of ceramic target damage is not obvious after impacted by two kinds of projectiles with different hardness at the same velocity.

1 National Natural Science Foundation of China (No.: 11072072)

F1.00072 The preheating effect on the dynamic strength of aluminum containing helium bubbles. BENNY GLAM, Soereq NRC, Yavne 81800, Israel, MOSHE STRAUSS, NRC Negev, Beer-Sheva 9001 Israel, SHALOM ELIEZER, DANIEL MORENO, Soereq NRC, Yavne 81800, Israel — The influence of helium bubbles or boron inclusions in an aluminum target is studied by plane impact experiments with a gas gun and VISAR diagnostic. The experiments were done for targets with initial temperatures of 25 °C and near melting at 600 °C. The Hugoniot elastic limit y HEL for all targets becomes substantially higher at 600 °C, related to the phonon drag mechanism at high strain rates and high temperatures. The y HEL and the elastic strain rate of the preheated samples with helium are lower than these without helium, therefore it is suggested that the helium is slowing down the mobile dislocation velocity. The spall strength for all targets becomes substantially lower at 600 °C. The spall strength of Al-10B with helium bubbles is significantly reduced in comparison to Al-10B without helium, while at 25 °C the spall strength is the same for both cases. The experiments are analyzed by using a one dimensional hydrodynamic simulation coupled to a spall model. The model applies an inertial Rayleigh type equation of motion for the void expansion with a viscosity term presenting the high strain rate plastic flow. The simulation results indicate that at room temperature the growing voids around boron inclusions are causing the spallation while the spall occurs in the preheated target with helium is dominated by growing helium bubbles.

F1.00073 Dynamic properties of a magnetic alloy Fe-Cr-Co. NATALIA NAUMOVA, SVETLANA ATROSHENKO, YURI SUDENKOV, NIKITA MOROZOV, XUEYIN SUN, IVAN SMIRNOV, 7-9, Universitetskaya nab., St.Petersburg, 199034, Russia — The high-strain-rate methods of materials were developed for dynamic strength investigations under microsecond durations of shock loads on the base of electrical explosion of conductors. The experimental investigations of dynamic properties for magnetic alloy Fe-Cr-Co under shock loads of microsecond duration (4-8) mks in the pressure range up to 20 GPa were carried out. The values of HEL and spall strength for these amorphous alloys were received. The results of microstructure analysis of saved specimens revealed essential differences in deformation mechanisms determining fracture and plasticity in these alloys under high-strain-rate.

F1.00074 Orientation-dependent response of nanovoids in Tantalum. DIEGO TRAMONTINA, Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, MS502.14MA Argentina, CARLOS RUESTES, Department of Mechanical and Aerospace Engineering, University of California, San Diego, La Jolla, CA 92093, USA, YIZHE TANG, Johns Hopkins University, Baltimore, MD 21212, USA, EDUARDO BRINGA, Consejo Nacional de Investigaciones Cientificas y Tecnicas. CABA. C1033AAJ Argentina — Defective BCC Tantalum monocrystals are expected to display a particularly rich behavior when stressed along different directions. Using molecular dynamics simulations, we model Ta monocrystals containing a single spherical void of different sizes, under uniaxial compression, for two different empirical potentials. Differences on the yield point, dislocation generation and plastic heating are observed depending on the void size and stress direction, as distinct slip systems are activated, resulting in a variety of dislocation structures and mobilities. We calculate plastic heating and dislocation densities, and compare results for different interatomic potentials.

F1.00075 Spall strength, dynamic elastic limit and fracture of ittrya dopped tetragonal zirconia. VLADIMIR MILYAVSKII, JIHT RAS, ANDREY SAVINYKH, IPCP RAS, THOMAS SCHLOTHAUER, TU Bergakademie Freiberg, EVGENY LUKIN, MUCTR, FELIX AKOPOV, JIHT RAS — Specimens of the ceramics based on zirconia partially stabilized by yttrium oxide of the composition of 97 mol % ZrO2 and 3 mol % Y2O3 were prepared. The densities of the specimens were 5.79 and 6.01 g/cc. The ceramics mainly have the tetragonal structure (93-98 wt. % of t-ZrO2). The mechanical action on the ceramic activates the transformation of the tetragonal phase into the monoclinic one: at the abrasive cutting or at the fracture by hammer shock, the content of the monoclinic phase is increasing. The same trend was observed in the specimens, recovered after stepwise shock compression up to 36, 52 and 99 GPa. It was found that shock compression do not initiates tetragonal-monoclinic phase transition directly, and this transition is caused by the destruction. Recovered specimens do not reveal any traces of the phase change which was observed by Mashimo et al. under the pressures 30-35 GPa (J. Appl. Phys. 1995. V. 77. P. 5069). Recording of the profiles of the free surface velocity of the specimens during single-stage shock compression allowed us to determine the dynamic elastic limit, as well as spall strength of the material versus maximal shock stress. In addition, the ceramics were subjected to the action of low temperatures. There were no significant changes in the specimens recovered after storage in liquid nitrogen and helium.

2 This work was supported by The Atomic Energy Corporation ROSATOM.

F1.00076 Effects of the grain size on the spall damage of copper. FENGQIU ZHANG, HONGQIANG ZHOU, Institute of Applied Physics and Computational Mathematics — The void nucleation equation of the NAG model is modified in the spall damage model for ductile metals, by considering the corresponding relation between grain size and potential nucleated void number. The simulation shows the influence of grain size on free surface velocity profile, qualitatively producing the consistent results determined experimentally by Escobedo (JAP,110,033513,2011).

F1.00077 The Influence of Grain-size on Dynamic Shear Localization in Thick Walled Copper Cylinders. ZEV LOVINGER, ZVI ROZENBERG, RAFAEL, DANIEL RITTEL, Technion - Israel Institute of Technology — Thick-Walled Cylinder collapse experiments were carried out on copper specimens to explore the influence of grain size on their spontaneous dynamic shear localization behavior. Average grain sizes of 20, 75, 200, and 300 μm, were achieved by means of heat treatments. Measuring the stress strain curve for the different coppers on the Kolsky-Bar apparatus showed no significant differences between the strength of these materials. This enabled us to pinpoint the microstructural influence on shear localization, excluding the possible effect of strength differences between the specimens. Experiments were conducted on a pulsed current generator using magnetic pressure as the driving force. Large plastic strains, of up to 1, were reached, for which preliminary results show the formation of intense twinning together with faint signs of localized shear bands in both fine and coarse grained specimens. We found at the inner surface of the specimens, where shear strains are the highest, a substantial layer of very fine grains followed by a layer with a very high density of twins. The weak appearance of shear bands in our copper specimens might be attributed to this fine grained layer, where shear bands initiate in this geometry, which we have not seen in other materials we tested such as Ti, Ti64 or stainless steel.

3 This research was funded by the ANPCyT project PICT2008-1325 and 06/M035 from SecTyP-U.N.Cuyo.
F1.00078 Multi-step Kolsky bar loading of metals which fail by adiabatic shear banding.

YECHESKEL ASHUAICH, ZVI ROSENBERG, CHEN AVINADAV, Rafael Advanced Defense Systems Ltd. — In a previous work we showed that thermal softening of materials in Kolsky bar tests can be eliminated by multiple step loading. Specimens made of metals which tend to undergo adiabatic shear banding fail at relatively low strains, due to local heating which enhances local reduction in strength. In this paper we present results from multi-step loading tests performed in our interferometry-based Kolsky bar, with specimens made of titanium and magnesium alloys and stainless steel. Multi-step loading should prevent the local heating of the specimen and, consequently, move the occurrence of shear banding to higher strains. However, our experiments showed that the specimens fail at about the same strains under multi-step and single loadings. Thus, the mechanism which is responsible to shear banding cannot be related to local heating and a new approach is needed to explain this phenomenon.

F1.00079 Two-dimensional Imaging Velocimetry of High-Strain Rate Deformation in Silicon.

SUZANNE ALI, Univ. of California, Berkeley. RAYMOND SMITH, Lawrence Livermore National Lab, CYNTHIA BOLME, Los Alamos National Lab, DAVID ERSKINE, PETER CELLIERS, JON EGGERT, Lawrence Livermore National Lab. JUE WANG, Princeton University, STEPHANIE BRYGGO, Commissariat à l’Énergie Atomique, BENJAMIN HAMMEL, None, GILBERT COLLINS, Lawrence Livermore National Lab, RAYMOND JEANLOZ, Univ. of California, Berkeley — The novel 2D-VISAR diagnostic that has been developed over the past few years has provided an unprecedented view into the details of material deformation during shock compression. Utilizing a two interferometer system with quadrant phase recording and an ultrashort laser pulse, a snapshot of the 2D velocity field of a shocked sample was obtained and the elastic and plastic breakout patterns were extracted. This diagnostic was used to measure the 2D velocity map of shock compressed single crystal silicon in three orientations, <100>, <110> and <111>. Varying the probe delay allowed us to track the evolution of complex deformation dynamics at the silicon interface. Characteristic breakout structures were found for each of the three orientations. The elastic breakout shapes demonstrated a dependence on the anisotropic wave speeds in the crystal and the plasticity was found to depend on the crystallographic slip planes.

F1.00080 Compaction model of damaged medium. IGNATOVA OLGA, RAEVSKIY VIKTOR, Retired, TSELIKOV IGOR'. None — At the present time difficulties emerge in the course of numerical simulation of high-rate processes of materials, accompanied by damage and compaction of defects (pores) under the action of compression waves. Compaction of defects formed by the action of pulsed tensile stresses is studied not sufficiently presently, and simplified mathematical models are used in calculations. The available compaction models are too complicated for their use in numerical procedures or they do not show all phenomena occurring at closing pores. A compaction model of a damaged medium is proposed in the present paper, which was based on the description of collapse of a single pore by taking into account elastic-plastic properties of a medium. To describe convergence of pores distributed with substance volume, a motion of one spherical cell was considered in an ideal-plastic incompressible medium. The analytical solution was obtained for the dependence of integral damage on pressure, shear strength and initial damage in this approximation. The equations were derived describing kinetics of compaction for the case of arbitrary pressure dependence on time and variable yield strength.

F1.00081 Experimental Comparison of Tantalum Material Strength between Single Crystal [100] and [111] Samples at High Pressure and Strain Rates¹. CHRISTOPHER PLECHATY, HYE-SOOK PARK, RÔB CAVALLO, ROBERT RUDD, SHON PRISBREY, BRIAN MADDUX, CHRISTOPHER WEHRENBERG, MARK MAY, BRUCE REMINGTON, Lawrence Livermore National Laboratory — Experiments were performed using the OMEGA laser to investigate the strength difference between single crystal [100] and [111] Ta samples at high pressure (1 Mbar), and high strain rates ($10^{10}-10^{11}$ s$^{-1}$). To achieve these pressures and strain rates in experiment without melting the sample, a quasi-inertotropic drive [1] was employed to drive the growth of pre-imposed sinusoidal perturbations on the surface of the Ta samples, via the Rayleigh-Taylor (RT) instability. By measuring the ripple amplitude using face-on high energy ($\sim$22 KeV) radiography [2], the strength of the Ta sample is inferred from the amount of RT growth observed [1]. Under these experimental conditions, the Ta material strength can be modeled by the Multiscale (MS) model [3], developed at LLNL. The value of the “Taylor Factor” (a MS model parameter), is thought to vary for [100] and [111] crystal orientations. To investigate this difference under these conditions, a comparison of the ripple growth was performed on the two samples for the same shot and drive conditions. [2] Barnes, J. F., et al., JAP 45, 727, (1974). [3] N. Barton et al., JAP 109, 073501 (2011).

¹This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

F1.00082 Multi-scale modeling of deformation and fracture of ceramic materials under dynamic loading. EVGENIYA SKRIPNYAK, VLADIMIR VLADIMIROVICH SKRIPNYAK, VLADIMIR ALBERTOVICH SKRIPNYAK, IRINA VAGANOVA, NATALIYA SKRIPNYAK, National Research Tomsk State University — The multi-scale approach to dynamic analysis of deformation and fracture, taking place in structured condensed matter show a great promise in prediction of the mechanical response for new materials. In present work the results of two-level simulations on deformation and fracture mechanisms for brittle materials subjected to impulse and shock-wave loadings are demonstrated. The dynamic effects occurring in structured representative volumes of the ceramics and the processes relating to damage and fracture of the ceramic materials with porous structures, ceramic composites and nanocomposites were modeled using the SPH methods. The grain, phase and porous structures were simulated in an explicit form. The presence of dispersed inclusions, dislocation substructures, nano- and micro-voids at the lower structural level were taking into account in an implicit form. The two-level model allows taking into account different relaxation and fracturing characteristic times at the different structural levels. This approach suggest to describe the relaxation process at the higher structural level in terms of integrated effect of the lower level processes. It is found that clusters of nano-voids in ceramic materials are the centers of damage nucleation. The presence of the clusters of nano-voids in ceramic materials subjected to dynamic loadings results in decrease of the Hugoniot elastic limit value.

F1.00083 A Lagrangian scheme based on characteristics theory for simulating two-dimensional flow on unstructured grids¹. LI TANG, YUTAO SUN, Institute of Applied Physics and Computational Mathematics — The paper presents a second order cell-centered finite volume method of 2D Lagrangian hydrodynamics based on semi-discrete framework. The velocity and pressure on the vertex of a cell are computed on the basis of the characteristics theory. Then, the two variables are used to compute the numerical flux through the cell interface by the trapezoidal integration rule. By combining with some reconstruction procedure, the method is extended to second order. An entropy modification strategy is proposed for simulating complex compressible flow. Several numerical experiments confirm good properties of convergence and symmetry of the method. The method permits large CFL number and can be applied on the structured and unstructured grids. It is also very robust in the multi-materials flow simulation.

¹Supported by NSFC No.11101046.

F1.00085 CO2 and CH4 clathrate hydrate under pressure. J.M. MENÉNDEZ, Departamento de Química Física y Analítica, Universidad de Oviedo, Oviedo, Spain, A. OTERO-DE-LA-ROZA, School of Natural Sciences, University of California, Merced, USA, F. IZQUIERDO, V. MUÑOZ, L. JIMENEZ, O. PRIETO-BALLESTEROS, Centro de Astrobiología (INTA-CSIC), Madrid, Spain, J.M. RECIO, Departamento de Química Física y Analítica, Universidad de Oviedo, Oviedo, SPAIN, MALTA CONSOLIDER TEAM — DFT first principles calculations have been performed to study the response to hydrostatic pressure of st-type CO2 and CH4 clathrate hydrates. Two kinds of simulations were carried out i) periodic crystalline structures were considered to optimize unit cell geometries, determine static equation of state parameters, and investigate the energetic stability of clathrates. Dispersion interactions have been accounted for by the exchange-hole dipole moment model recently implemented for solid state calculations. It is found that, gas filling is a stabilization process independent on the guest molecule. However, while CH4 shows no preference for the size of the cage, the effect of stabilization is more pronounced when CO2 is in 5146 cages. Pressure also favors stabilization of both molecules, with CO2 being more sensitive than methane. ii) Molecular calculations using finite clusters were also carried out. At selected geometries, vibrational frequencies and intensities have been computed for all the gas-cage combinations. A change in the vibrational modes due to the confinement of the guest molecules is revealed. However, pressure barely affects the Raman/IR spectrum of the clathrate. These theoretical findings will be compared with experimental data already in progress.

F1.00086 Patterning in stress: a new insight into the deformation behavior of polycrystalline materials. PAMELA BURNLEY, University of Nevada, Las Vegas — The distribution of stress and strain in plastically deforming polycrystalline materials is widely observed to be heterogeneous and has so far evaded simple characterization. While elastic plastic and visco plastic self-consistent models (with assumption that the Schmid factor governs slip) enjoy some success in predicting macroscopic behavior, the distribution of strain between constituent grains is not well predicted by the Schmid factor. This lack of correlation is caused by differences between the macroscopic stress state and the local stress state at each crystal due to the mechanical interconnections of neighboring grains. Using 2D plane strain finite element models of large ensembles of grains, I show that the distribution of stress in a polycrystal forms patterns that are broadly reminiscent of those associated with phenomena that are governed by percolation theory. The pattern of stress transmission is related to the degree of heterogeneity in and statistical distribution of the elastic and plastic properties of the constituent grains in the aggregate. For a highly heterogeneous polycrystals, the patterns are similar to force chains observed in granular materials. For a more homogeneous polycrystal, the density of force chains is greater and the degree of stress concentration in them is less. Understanding stress patterning will be critical for linking the macroscopic rheology of polycrystalline materials to the single crystal elastic and plastic properties of their constituent crystals.

F1.00087 Effect of pressure on electronic & optical properties of Cadmium Chalcogenides. DHARMIBIR SINGH, PIET, Samalkha, Panipat, Haryana, INDIA, PAWAN KUMAR, J.C.D.M. College of Engineering, Sirsa, Haryana, INDIA — We report effect of pressure on electronic & optical properties of Cadmium Chalcogenide. The theoretical computational study of these materials are done out using the full-potential linear augmented plane wave (FP-LAPW) method. In this approach the Generalized-gradient-approximation (GGA) is used for the exchange–correlation (XC) potential. We have calculated the equilibrium lattice constant, electronic band structure dispersion, total & partial density of electron states, band gap, bulk modulus, and its pressure derivative. The calculated parameters are found in good agreement with experimental and other theoretical results. Furthermore, optical constants such as dielectric functions, refractive indices, reflectivity, absorption coefficient, optical conductivity, loss functions of stable Cadmium chalcogenide S were calculated for photon energies at ambient & high pressure.

F1.00088 Refractive index of K9 Glass under Shock Loading. CHANGMIN HU, XIANG WANG, LINGCANG CAI, CAGLI LIU, Institute of Fluid Physics, China Academy of Engineering Physics, Miyang, 621900, China — We study K9 glass refractive index under shock loading conducted on powder gun, all experimental tests are plate impact loading. The impact velocetry range from 300m/s to 1200m/s, and the measure method is laser interferometer Photon Doppler Velocimetry(PDV) to measure the particle velocity both at the impact interface and free surface, The shock pressure from 2GPa to 8GPa, values for refraction are found from velocity corrections that must be made to account for refraction-index changes in the K9 glass due to shock wave motion. Experiment results show that refraction-index of K9 glass changes with the shock pressure in line relations, it can be as measure window to study the interesting materials under 10GPa during the shock loading.

F1.00089 XMCD investigation of Rare Earth Metal at high pressure conditions. LUCIE NATAF, FRANCOIS SAUDELET, Synchrotron SOLEIL – The X-ray Magnetic Circular Dichroism is a selective magnetic probe for high pressure studies. Nowadays, XMCD under pressure is usually employed, mainly on 3d and 5d metal systems. We will present new results on Rare Earth metals. Up to now, most of the pressure works are devoted to the structural properties of RE. However, only a few works deal with the pressure effect on their magnetic properties. RE, having high magnetic moment and large anisotropy, are commonly used for practical applications. Nevertheless, their magnetic ordering temperature is below RT. Adding transition metals solves this limitation: the alloys then present the advantages of RE and the high magnetic ordering temperature of TM. To optimize the properties of these systems, a pressure study may be a better way than an empirical investigation. Interpreting the XMCD signal at the L three edges of RE is very difficult since many contributions are involved. The important role of the 4f-5d interactions has to be taken into account and the quadrupolar transitions will be critical for linking the macroscopic rheology of polycrystalline materials to the single crystal elastic and plastic properties of their constituent crystals.

F1.00090 The Bactericidal Effect of Shock Waves. JAMES LEIGHS, GARETH APPLEBY-THOMAS, DAVID WOOD, MICHAEL GOFF, AMER HAMEED, Cranfield University, PAUL HAZELL, The University of New South Wales — There are a variety of theories relating to the origins of life on our home planet, some of which discuss the possibility that life may have been spread via inter-planetary impacts. There have been a number of investigations into the ability of life to withstand the likely conditions generated by asteroid impact (both contained in the impactor and buried beneath the planet surface). Previously published data regarding the ability of bacteria to survive such applied shock waves has produced conflicting conclusions. The work presented here used an established technique, in combination with a single stage gas gun to shock load and subsequently recover Escherichia coli populations suspended in a phosphate buffered saline solution. Peak pressure across the sample region was calculated via numerical modelling, validated via Heterodyne velocimetry measurements. Survival data against peak sample pressure for recovered samples is presented alongside control tests.
F1.00091 Imaging velocity interferometer system for any reflector based on Shen Guang-III prototype laser facility. WANG FENG, PENG XIAOSHU, ZHANG RUI, Research Center of Laser Fusion, CAEP. — The imaging velocity interferometer system for any reflector (VISAR) has been introduced in this report for shock-timing experiment in inertia confined fusion (ICF). Some important techniques have been provided, including the probe laser with single mode and shaped capability, imaging technique with high resolution and calibration character. The new target design can be used widely after analyzing the interaction of laser and target. Then the blanking effect on the signal can be avoided. Without the quartz window effect, the new target concept with the reflected design can be provided to do the Deuterium-tritium (DT) material experiment. After using this concept, the fourth shock can be diagnosis easily in shock-timing experiment. Since the one dimension Fourier transform method (FTM) may occur the data loss, the new unwrap algorithm should be developed. The new flood algorithm with high confidence has been programmed. Although the fringe contrast of VISAR is very low, the unwrapping phase map can be satisfied. The space resolution of imaging VISAR is 5 μm, and the time resolution is 10ps ~ 30ps. The uncertainty is less than 2%, which has reached the international level.


F1.00093 Underwater Shock Response of Air-Backed Thin Aluminum Alloy Plates: An Experimental and Numerical Study. PENG REN, WEI ZHANG, Harbin Institute of Technology — Studies on dynamic response of structures subjected to underwater explosion shock loading are of interest to ship designers. Understanding the deformation and failure mechanism of simple structures plays an important role in designing a reliable structure under this kind of loading. The objective of this combined experimental and numerical study is to analyze the deformation and failure characteristics of 5A06 aluminum alloy plates under underwater shock loading. Some non-explosive underwater blast loading experiments were carried out on air backed circular plates of 2mm thickness. The deformation history of the clamped circular plate was recorded using a high speed camera and the deflections of specimens at different radii were measured in order to identify deformation and failure modes. In the finite element simulations, the strength model of 5A06 aluminum alloy is considered using the slightly modified Johnson-cook mode to describe structure deformation. Good agreement between the numerical simulations and the experimental results is found. Detailed computational results of each scenario are offered to understand the deformation and failure mechanism.

F1.00094 Mesoscale Probing of Local Perturbations in PBX-driven Liners. IGOR PLAKSIN, ADAI, Univ of Coimbra, Portugal. RAAFAT GUIRGUIS, NSWC-IH, LUIS RODRIGUES, RICARDO MENDES, SVYATOSLAV PLAKSIN, ADAI, Univ of Coimbra, ADAI, UNIV OF COIMBRA AND NSWC-IH COLLABORATION — Efforts are aimed on experimental studies of how to improve a dynamic performance of the shaped charge jet. We postulated four basic elements to the problem: (1) The fluctuations in properties inherent in PBXs cause kinetic localizations in the detonation reaction zone (DRZ) structure, which cause (2) perturbations in the detonation products velocity and pressure, which induce (3) Perturbations in the response of the PBX-driven liner; and (4) Local perturbations/instabilities in liner are amplified during its collapse phase causing micro-fragmentations and ejected debris from the cumulative jet at initial stage, and then the incoherence and premature breakup of the resulting shaped charge jet. Spatially-resolved scenarios of each of phenomena (1-4) were obtained in experiments with copper-liners and HMX-based PBXs manufactured on maximum packing density of crystalline constituents, in which the DRZ-induced perturbations were recorded and quantitatively measured in the mesoscale range with application of the 96-channel optical analyzer MCOA-UC. Obtained experimental evidence is indicative that ejecta from the DRZ and ejecta-driven detonation cells are dominating in wide spectrum perturbations translated to a PBX-driven liner.

F1.00095 Table-top Generation and Spectroscopic Study of ~10 TPa High-Energy Density Materials with C_{60} Hypervelocity (v ~ 100 km/s) Impact. YOUNG BAE, Y.K. Bae Corporation — Intense bursts of soft x-rays were discovered by Bae et al. in hypervelocity (v ~ 100 km/s) impact of bio and water nanoparticles at the Brookhaven National Lab (BNL) in 1994. In the experiment, the nanoparticles were directly generated by a laser pulse and detected by Si particle detectors that were located outside the shock wave. Energy deposition measurements through thick films revealed that the impact generated pressures were ~10 TPa, and the photon energies in the range of 75-100 eV for Si targets. The conversion efficiency from the kinetic energy to the radiation energy was unexpectedly high, ~38%, which was attributed to Dicke Superradiance of collective quantum states in High-Energy Density Materials (HEDM), Metastable Innershell Molecular States (MIMS). This talk presents recent experimental results obtained in a table-top apparatus completely different from and orders of magnitude smaller than that at BNL. In the new setup, hypervelocity (v 100 km/s) C60− ions impacted on Al targets, and the impact generated soft x-rays were detected off-axis and analyzed using three Si photodiode detectors with selective energy response curves. The photon energy was determined to be ~70 eV with the kinetic-energy to photon-energy conversion efficiency of ~35% in confirmation of the results by Bae et al. BNL. The present results demonstrate a new way of generation and spectroscopic study of HEDM with pressures exceeding 10 TPa, and show the pathway to scaling up the soft x-ray generation method for a wide range of applications from lithography to inertial fusion.

1National Natural Science Foundation of China (NO.11072072)

2ADAI, Univ of Coimbra, Portugal
Characterization of Viscoelastic Materials for Low-Magnitude Blast Mitigation. SUSAN BARTYCZAK, WILLIS MOCK, Naval Surface Warfare Center Dahlgren Division — Recent preliminary research indicates that exposure to low amplitude blast waves, such as from IED detonation or multiple firings of a weapon, causes damage to brain tissue resulting in Traumatic Brain Injury (TBI) and Post Traumatic Stress Disorder (PTSD). Current combat helmets are not sufficiently protecting warfighters from this danger and the effects are debilitating, costly, and long-lasting. The objective of this research is to evaluate the blast mitigating behavior of current helmet materials and new materials designed for blast mitigation using a test fixture recently developed at the Naval Surface Warfare Center Dahlgren Division for use with an existing gas gun. A 40-mm-bore gas gun is used as a shock tube to generate blast waves (ranging from 5 to 30 psi) in a test fixture mounted at the gun muzzle. A fast opening valve is used to release helium gas from a breech which forms into a blast wave and impacts instrumented targets in the test fixture. Blast attenuation of selected materials is determined through the measurement of pressure and accelerometer data in front of and behind the target. Materials evaluated in this research include 6001-T6 aluminum, polyurea 1000, Styrofoam, and Sorbothane (durometer 50, shore 00). The experimental technique, calibration and checkout procedures, and results will be presented.

Measuring Three-Dimensional Deformation with Surface-Imaging ORVIS. MARCIA COOPER, WAYNE TROT, JILL MILLER, Sandia National Laboratories — With growing interest in understanding heterogeneous material phenomena under shock compression and the advancement of computational methods, three-dimensional data suitable for model validation and scientific pursuit is needed. The optically recording velocity interferometer system (ORVIS) is a velocity interferometer that measures the apparent motion of a set of parallel interference fringes. Initially demonstrated for collecting one-dimensional data at a point using a streak camera and a focused laser spot, line-imaging ORVIS is a useful extension for the collection of two-dimensional data using a streak camera and a laser light sheet. We extend ORVIS operation further to a surface-imaging mode for collecting three-dimensional data using a framing camera and an expanded region of laser illumination. In surface-imaging mode, snapshots of surface velocity across a cross-sectional area are collected at regular time intervals and combined to yield the surface velocity history. Data collected with surface-imaging ORVIS applied to several model problems will be presented along with a discussion of the analysis methodology and some experimental challenges.

VISAR ‘cross-hairs’: Simultaneous perpendicular line-imaging VISAR. JOHN WINTERS, SIMON BLAND, SAMUEL STAFFORD, DANIEL EAKINS, DAVID CHAPMAN, Institute of Shock Physics, Imperial College London — Often the velocity measured at the rear surface of a dynamic compression target varies spatially, caused for instance by the tilt/curvature of a gas gun flyer, asymmetries in the magnetic field on a pulsed power driven experiment, or mesoscale heterogeneous targets. One way to monitor this in an experiment is to employ multiple point velocity techniques, but even with multiplexing this can become expensive in terms of hardware, in particular high speed sensors and scope channels. We report on the development of a multi-beam VISAR system that provides a spatial velocity along two orthogonal directions. Cylindrical optics are used to project a set of cross-hairs onto the target, maximising the use of input laser light. We describe the image relay and interferometer configuration, along with an evaluation of system resolution. This ‘quasi’ two dimensional system will become one of the principal diagnostics on the MACH (Mega Ampere Compression and Hydrodynamics) facility, where the multi-axis measurement will help optimise strip-line design to achieve uniform ramp compression of targets.

Single-Shot Ellipsometry for the Z-Machine. SEAN GRANT, AARON BERNSTEIN, University of Texas at Austin, TOM AO, JEAN-PAUL DAVIS, Sandia National Laboratories, TODD DITMIRE, University of Texas at Austin, DANIEL DOLAN, DAWN FLICKER, Sandia National Laboratories, JUNG-FU LIN, NATHAN RILEY, University of Texas at Austin, CHRIS SEAGLE, Sandia National Laboratories — We have developed a single-shot ellipsometry diagnostic capable of taking time-resolved measurements. A comparison of dielectric constants obtained using this method with those from a standard spectroscopic ellipsometry technique showed good agreement when used to measure a static Au sample. The ellipsometer is being designed for use on the Z-machine at Sandia National Laboratories to measure the conductivity of Fe at pressures and temperatures of the Earth’s core.

Termination and hydration of ultramafic mineral surfaces: Forsterite (010) and Diopside (010) surfaces. HONGPING YAN, CHANGYONG PARK, Carnegie Institution of Washington — The weathering and hydrous alteration processes of ultramafic rocks (serpentinitization) are known to contribute to abiotic hydrocarbon generation in near surface region of the planet. Atomic level characterization of the interface between water and mineral surface, which plays crucial roles in mineral weathering and dissolution, is highly demanded to better describe the processes in molecular scale. We use in-situ high-resolution X-ray reflectivity to examine the natural forsteritic olivine (010) surface and diopside (010) surface in aqueous environments. By modeling the electron density profile in surface normal direction and fitting the measured data with least-square method, the atomic structures of hydrated mineral surfaces are depicted. We found, for alumina polished forsterite surface under acidic environment, a homogenous termination with about half of the magnesium depleted and replaced with possibly the hydronium ions. In contrast, the silica polished forsterite does not show such homogenous surface, as confirmed by ex-situ Atomic Force Microscopy measurements. In comparison, the diopside (010) surface is naturally grown without any polishing but, interestingly, it shows qualitatively identical features to forsterite (010) in terms of the termination and the first adsorbed water structures. These results indicate a common chemical characteristic of these mineral surfaces interacting with water, despite the distinguishing silica ratios and silicate structures they have.

Deformation of an Iron-based bulk metallic glass at high strain-rates. GAURI KHANOLKAR, VERONICA ELIASSON, University of Southern California — Bulk metallic glasses (BMG) are multi-component, amorphous alloys that have garnered recent interest due to their high strength and hardness. Although extensive work on their response to quasi-static, uniaxial loading exists, the behavior of BMG, especially iron-based ones, under dynamic shock loading has not been fully explored. In this work, we conduct reverse-Taylor plate impact experiments of an iron-based alloy commonly known as SAM2X5 at impact velocities up to 300 m/s using a gas gun, and at higher velocities of up to 2000 m/s using a powder gun, in order to determine its response to high strain-rate loading. Resulting deformation is observed under a Scanning Electron Microscope. Experiments at higher velocities are instrumented using a Velocity Interferometer System for Any Reflector. In addition, a Zr-based BMG commonly known as Vitreloy 106a will be also subjected to the same impact conditions, in order to compare its dynamic response with that SAM2X5. Since Iron alloys have higher densities than Zr ones (7.6 g/cc compared with 6.7 g/cc), it is expected to result in more superior strength properties for the former. A comparison of fracture morphologies and differences in spall strengths, Hugoniot elastic limits, magnitudes of strain-to-failure etc are studied.

The effect of varying aspect ratios on the low strain rate behaviour of metals and polymers. AMNAH KHAN, JENS BALZER, WILLIAM PROUD, Institute of Shock Physics, Imperial College London — This poster looks at the effect of varying aspect ratios, from 1:4 to 3:1, on a number of different materials, including aluminium and polycarbonate. A range of strain rates ($10^{-4}$ s$^{-1}$ to $10^{-3}$ s$^{-1}$) is achieved using quasi-static Instron equipment, drop weight machines and Split Hopkinson Pressure Bars. The mechanical behaviour is discussed, and high-speed video used to further the analysis.

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Defense Threat Reduction Agency

Thanks to AWE for their continued funding and support.
F1.00103 Lateral stress evolution in Chromium Sulfide. OREN PETEL, McGill University, Department of Mechanical Engineering, Montreal, QC H3A 0C3, Canada; GARETH APPLIEBY-THOMAS, AMER HAMEED, Cranfield Defence and Security, Cranfield University, Shrivenham, Swindon, SN6 8LA, United Kingdom; ALEXANDER CAPOZZI, DAVID FROST, McGill University, Department of Mechanical Engineering, Montreal, QC H3A 0C3, Canada; PAUL HAZELL, School of Engineering and Information Technology, UNSW Canberra, University of New South Wales, Northcott Drive, Canberra, ACT 2600, Australia. — In this paper the shock response of chromium sulfide, a cermet of potential interest as a matrix material for ballistic applications, has been investigated. Compacts with a Chromium-Sulfur ratio of 1:15:1 were investigated via the plate-impact technique. These experiments allowed the material to be loaded under a one-dimensional state of strain. Embedded manganese stress gauges were employed to monitor the temporal evolution of longitudinal and lateral components of stress. Comparison of these two components has allowed assessment of the variation of material shear strength both with impact pressure/strain-rate and time. Interestingly tentative evidence of what appeared to be an elastic-plastic transition was noted on the lateral traces, despite the absence of a lateral shock.

F1.00104 Shock response of 7068 aluminium alloy. DAVID CHAPMAN, DANIEL EAKINS, WILLIAM PROUD, Institute of Shock Physics, Imperial College London, London, SW7 2AZ, United Kingdom. — Aluminium alloys are widely employed throughout the aerospace and defence industries due to their high specific strength. Aluminium alloy 7068, often described as the ultimate aluminium alloy was developed by Kaiser Aluminium in the mid-1990s and is the strongest aluminium commercially produced. There remains little published data on the response of this micro-structurally anisotropic alloy to dynamic loading. As part of an investigation of the high-rate mechanical properties of Al 7068, a series of plate-impact experiments using a novel meso-scale planar impact facility and a more conventional large bore gas gun were undertaken. The evolution of the elastic-plastic shock wave and spall strength as a function of sample thickness and specimen orientation were investigated using optical velocimetry (line-VISAR, PDV) techniques. Planar shock wave experiments were conducted on specimens several 100 microns to several millimetres thick cut from either parallel or perpendicular to the extrusion direction.

F1.00105 Hugoniot-based equations of state for two filled EPDM rubbers. ADAM H. PACHECO, DANA M. DATTELBAUM, Los Alamos National Laboratory, E. BRUCE ORLER, Virginia Tech, R.L. GUSTAVSEN, Los Alamos National Laboratory. — The shock response of silica filled and Kevlar filled ethylene-propylene-diene (EPDM) rubbers was studied using gas gun-driven plate impact experiments. Both materials are proprietary formulations made by Kirkhill-TA, Brea CA USA, and are used for ablative internal rocket motor insulation. Two types of experiments were performed. In the first, the filled-EPDM sample was mounted on the front of the projectile and impacted a Lithium Fluoride (LiF) window. The Hugoniot state was determined from the measured projectile velocity, the EPDM/LiF interface velocity (measured using VISAR) and impedance matching to LiF. In the second type of experiment, electromagnetic particle velocity gauges were embedded between layers of filled-EPDM. These provided in situ particle velocity and shock velocity measurements. Experiments covered a pressure range of 0.34 – 14 GPa. Hugoniot-based equations of state were obtained for both materials, and will be compared to those of other filled elastomers such as silica-filled polydimethylsiloxane and adiprene.

F1.00106 Tuning the Electrical and Optical Properties of MoS2 under High Pressure. AVINASH P. NAYAK, Department of Electrical & Computer Engineering, University of Texas at Austin, JIE ZHU, JUNG-FU LIN, Jackson School of Geosciences, University of Texas at Austin, DEJI AKINWANDE, Department of Electrical & Computer Engineering, University of Texas at Austin. — Transition metal dichalcogenides (TMDCs), such as molybdenum disulfide (MoS2), has been of recent interest to many theoretical and experimental studies. MoS2 has served as a potential material for optoelectronic and field-effect-transistors (FETs) with high on/off ratios (up to 105). MoS2 is composed of quasi-two-dimensional sheets that are stacked on top of one another where each monolayer is tri-layered with a transition metal, molybdenum, in the middle that is covalently bonded to a chalcogen atom, sulfur, located on the top and bottom of the layers. These layers are separated by weak van der Waals (vdW) forces along the c-axis which makes the properties of MoS2 anisotropic. Having control over the electronic properties, and therefore, the band-gap of MoS2, allows for a wide range of applications from electrochemical devices to tunable photo-detectors to be adopted. We demonstrate the electronic phase transition of MoS2 from semiconducting to a metallic state at ~15GPa. The electronic transport properties in the semiconducting region (lower pressures) exhibits a shockley-like behavior while in the metallic region (higher pressures), we observe ohmic transport. We also examine the light-induced electronic properties by creating optical switches under pressure in greater detail. This photo-current behavior of MoS2 allows for optical switches with three order decrease in turn-on time. We examine the change in the activation energy, optical Raman, XRD, and resistance, by inducing pressure to MoS2 up to 35 GPa.

F1.00107 Three-dimensional constitutive model for shock-induced phase transition with N transforming phases. ZHIPING TANG, YANGBO GUO, Univ. of Sci. and Tech. of China. — Phase transitions are commonly controlled by pressure, shear and temperature. In this paper we established 3D incremental constitutive equations for both “stress-induced” and “strain-induced” phase transitions with N transforming phases based on the Gibbs free energy of each phase, which can describe the dynamic deformation behavior of mixed phase. An evolution equation was established considering the over driving force and the growing space in the transition process. The critical criteria, the constitutive equation of mixed phase and the evolution equation constitute the whole constitutive model. The α-ε transition simulation of iron with the present model coincides qualitatively with the experimental result.

F1.00108 High pressure synthesis and properties of Sr2CuO3+δ. Q.Q. LIU, Institute of Physics CAS.

F1.00109 Intrinsic ferroelectric polarization study of RMnO3. S.M. FENG, Institute of Physics CAS.

F1.00110 Numerical Simulation of Shear Bands in Depleted Uranium. JEEYEON PLOHR, Los Alamos National Laboratory.
Since the pioneering experimental studies of Percy W. Bridgman, an enormous progress in high pressure research has resulted in tremendous gains of knowledge about materials behavior over a wide range of pressures. Today’s experimental studies of solids take advantage of numerous developments in pressure-cell techniques and advances in analytical methods that utilize synchrotron x-ray radiation (diffraction as well as inelastic scattering), low-temperature optical spectoscopies, and synchrotron infrared spectroscopy. The subjects of interest range from fundamental questions about phase stability, crystal structure formation, and the nature of interatomic bonding to illuminating the interplay between subtle changes in atomic arrangements, electron delocalization, magnetism, and superconductivity. In this presentation I intend to briefly highlight (i) selected contributions of diamond-cell-based research to understanding electrons, phonons, and other quasiparticles in “conventional” semiconductors and (ii) the more recent surprises in the field of phase stability of non-transition metals. The main focus will be on structural and electronic properties of transition metal compounds located near the insulator-metal borderline. There, the orbital physics of perovskite-related titanates and vanadates (pressure-induced rearrangement of t2g states and related insulator to metal transitions) has attracted attention. Pressurizing multiferroic spinels leads to structural diversity and oxidation state changes when entering into a metallic regime. And by revisiting one of the cuprate superconductors it reveals polymorphism which may call for a reinterpretation of the Tc maximum induced by pressure. These examples from experiment indicate where the advanced models of correlated electron systems are expected follow up on the considerable success of theoretical physics in accounting for or predicting pressure effects in solids.

Tuesday, July 9, 2013 9:15AM - 10:15AM – Session H1 TM Computational Shock Compression of Single/poly Crystals Grand Ballroom I - Keith Gonthier, Louisiana State University

9:15AM H1.00001 Shock compression of Ta single crystals with dislocation sources1 . DIEGO TRAMONTINA, Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, MS502JMA Argentina, RAMON RAVELO, Physics Department and Materials Research Institute, University of Texas, El Paso, TX 79968, EDUARDO BRINGA, Consejo Nacional de Investigaciones Cientificas y Tecnicas, CABA, CI033AAJ Argentina — We present non-equilibrium molecular dynamics (NEMD) simulations of shock wave compression of line Tantalum single crystals including pre-existing defects, which act as dislocation sources. We use the new embedded atom model (EAM) potential presented by Ravelo et al. [Ravelo et al., SCMM2011 paper], developed for shock-wave simulations. We study the nucleation and evolution of doubletains and twins as a function of shock pressure and loading ramp time. We find a large dependence of the HEL (Hugoniot Elastic Limit) on strain rate. We compare the resulting dislocation densities and dislocation structures to existing experimental results on recovered samples.

This research is funded by the ANPCyT project PICT2008-1325 and 06/M035 from SecTyP-U.N. Cuyo.

9:30AM H1.00002 Shock Compression of Beryllium Single Crystals: Time-Dependent, Anisotropic Elastic-Plastic Response , J.M. WINEY, Y.M. GUPTA, Washington State University — To gain insight into inelastic deformation mechanisms in shocked Be single crystals, wave propagation simulations were performed for crystals shocked along the c-axis, a-axis, and other crystal directions to peak stresses reaching 7 GPa. The simulations utilized a time-dependent, anisotropic material model that incorporated dislocation dynamics and deformation twinning based descriptions of inelastic deformation. The simulation results showed good qualitative agreement with the measured wave profiles [Pope and Johnson, J. Appl. Phys. 46, 720 (1975)], including features arising from wave mode coupling due to the highly anisotropic inelastic response of Be. The measured wave profiles can be understood in terms of dislocation slip along basal, prismatic, and pyramidal planes, together with deformation twinning. Our results provide insight into the complex nature of inelastic deformation in shocked Be, and are also expected to be valuable for understanding the anisotropic inelastic response of analogous hcp metals subjected to shock compression. Work supported by ARL and DOE/NNSA.

9:45AM H1.00003 An Overview of Mesoscale Material Modeling with Eulerian Hydrocodes1 , KARL OLNEY, University of California, San Diego — Eulerian hydrocodes were originally developed for simulating strong shocks in solids and fluids, but their ability to handle arbitrarily large deformations and the formation of new free surfaces makes them attractive for simulating the deformation and failure of materials at the mesoscopic scale. A summary of some of the numerical techniques that have been developed to address common issues for this class of problems is presented with the shock compression of powdered used as a model problem. Achieving the correct packing density with the correct statistical distribution of particle sizes and shapes is, in itself, a challenging problem. However, since Eulerian codes permit multiple materials within each element, or cell, the material interfaces do not have to follow the mesh lines. The use of digital image processing to map the pixels of micrographs to the Eulerian mesh has proven to be a popular and useful means of creating accurate models of complex microstructures. Micro CT scans have been used to extend this approach to three dimensions for several classes of materials. The interaction between the particles is of considerable interest. During shock compression, individual particles may melt and form jets, and the voids between them collapse. Dynamic interface ordering has become a necessity, and many codes now have a suite of options for handling multi-material mechanics. True contact algorithms are now replacing multi-material approximations in some cases. At the mesoscale, material properties often vary spatially due to sub-scale effects. Using a large number of material species to represent the variations is usually unattractive. Directly specifying the properties point-wise as history variables has not proven successful because the limiters in the transport algorithms quickly smooth out the variations. Circumventing the limiter problem is shown to be relatively simple with the use of a reference configuration and the transport of the initial coordinates.

1 Research supported by Los Alamos National Laboratory and the Office of Naval Research

Tuesday, July 9, 2013 9:15AM - 10:45AM – Session H2 CM.2 Phase Transitions: Tantalum and Molybdenum Grand Ballroom II - Carl Greeff, Los Alamos National Laboratory

9:15AM H2.00001 Structures, properties, and phase Transformations of Ta at high pressures and temperatures , DENNIS KLUG, National Research Council of Canada, YANSUN YAO, University of Saskatchewan, NRC-UNIVERSITY OF SASKATCHEWAN COLLABORATION — High pressure structures and phase transformations of dense Ta were studied with several theoretical methods to address recent controversies regarding the properties of this element. The objective is to characterize the structure of Ta at high temperatures and pressures where possible phase transitions could occur and have been reported. The techniques employed include structure search methods and the metadynamics method based on density functional theory, together with a detailed analysis of the mechanical and dynamical properties of candidate structures the may be stable near the melting temperature of Ta and to pressures up to several TPa which are currently obtainable in shock-compression experiments. This includes a characterization of anharmonic effects on the dynamical and mechanical stability of Ta over the temperature range from 0 K to the melting temperature.

9:30AM H2.00002 Structures, properties, and phase Transformations of Ta at high pressures and temperatures , J.M. WINEY, Y.M. GUPTA, Washington State University — To gain insight into inelastic deformation mechanisms in shocked Be single crystals, wave propagation simulations were performed for crystals shocked along the c-axis, a-axis, and other crystal directions to peak stresses reaching 7 GPa. The simulations utilized a time-dependent, anisotropic material model that incorporated dislocation dynamics and deformation twinning based descriptions of inelastic deformation. The simulation results showed good qualitative agreement with the measured wave profiles [Pope and Johnson, J. Appl. Phys. 46, 720 (1975)], including features arising from wave mode coupling due to the highly anisotropic inelastic response of Be. The measured wave profiles can be understood in terms of dislocation slip along basal, prismatic, and pyramidal planes, together with deformation twinning. Our results provide insight into the complex nature of inelastic deformation in shocked Be, and are also expected to be valuable for understanding the anisotropic inelastic response of analogous hcp metals subjected to shock compression. Work supported by ARL and DOE/NNSA.

9:45AM H2.00003 An Overview of Mesoscale Material Modeling with Eulerian Hydrocodes1 , KARL OLNEY, University of California, San Diego — Eulerian hydrocodes were originally developed for simulating strong shocks in solids and fluids, but their ability to handle arbitrarily large deformations and the formation of new free surfaces makes them attractive for simulating the deformation and failure of materials at the mesoscopic scale. A summary of some of the numerical techniques that have been developed to address common issues for this class of problems is presented with the shock compression of powdered used as a model problem. Achieving the correct packing density with the correct statistical distribution of particle sizes and shapes is, in itself, a challenging problem. However, since Eulerian codes permit multiple materials within each element, or cell, the material interfaces do not have to follow the mesh lines. The use of digital image processing to map the pixels of micrographs to the Eulerian mesh has proven to be a popular and useful means of creating accurate models of complex microstructures. Micro CT scans have been used to extend this approach to three dimensions for several classes of materials. The interaction between the particles is of considerable interest. During shock compression, individual particles may melt and form jets, and the voids between them collapse. Dynamic interface ordering has become a necessity, and many codes now have a suite of options for handling multi-material mechanics. True contact algorithms are now replacing multi-material approximations in some cases. At the mesoscale, material properties often vary spatially due to sub-scale effects. Using a large number of material species to represent the variations is usually unattractive. Directly specifying the properties point-wise as history variables has not proven successful because the limiters in the transport algorithms quickly smooth out the variations. Circumventing the limiter problem is shown to be relatively simple with the use of a reference configuration and the transport of the initial coordinates.

1 Research supported by Los Alamos National Laboratory and the Office of Naval Research
9:30AM H2.00002 Melting curve of Ta from the modified Z method in molecular dynamics simulation1, WANG SHUAICHUANG, LIU HAIFENG, ZHANG GONGMU, SONG HAIFENG, TANG LI, IAPCM (Institute of Applied Physics and Computational Mathematics), IAPCM TEAM — Our recently proposed modified Z method to calculate the melting curve of metals has an obvious feature that a system can run naturally into its steady solid-liquid coexistence state from a perfect solid configuration in one running process. The method has been proved to be successful for face-centered cubic metals. Now we examine its validity for the melting curve of body-centered cubic metals, Ta as an example. A steady solid-liquid coexistence state can still be achieved for a system with only about 1000 atoms. The melting temperature and pressure results of Ta, extracted from the coexistence state, are in good agreement with those of the two-phase method in the literature.

9:45AM H2.00003 Rarefaction wave propagation and longitudinal sound velocities in shock compressed tantalum, ROBERT SCHARFF, Los Alamos National Laboratory — The purpose of this work is to investigate the bcc to hexagonal structural phase transition recently reported for shock compressed tantalum. Longitudinal sound velocities were obtained using a velocimetric diagnostic to record the shock and rarefaction wave arrival times at the sample/anvil interface in the reverse-ballistic plate impact geometry. This approach allows for the determination of the sound speed as a function of pressure and is sensitive to volume changes associated with phase transition behavior. The authors demonstrate that if elastic – plastic wave interactions are correctly determined, then the high pressure structural phase transition that has been previously reported is notably absent.

10:15AM H2.00004 The compressibility and sound velocity measurements of molybdenum up to ~0.7 TPa, CHENGDA DAI, XIANG WANG, XIULU ZHANG, QINGSONG WANG, KE JIN, YE TAN, HONGXING SONG, FENG XI, JIANBO HU, HUA TAN, Institute of Fluid Physics, CAEP — The compressibility (Hugoniot) and sound velocity data of matter are of particular importance for constructing high-pressure equation of state and/or detecting phase transitions. In this presentation, we report the Hugoniot measurements of Mo up to ~0.7 TPa performed on a gas gun. A hypervelocity flyer launcher was fixed on a two-stage gun muzzle for a graded-density impactor to drive Ta secondary flyer up to ~10 km/s. The simultaneous measurements of Ta flyer velocity and shock wave velocity of Mo in each shot yielded a Hugoniot data pair. The obtained results are in a good agreement with available data. The sound velocities of Mo were also measured under shock pressure from ~60 GPa to ~160 GPa using a backward or forward impact geometry based on rarefaction overtake method. The extracted data smooth in tendency the knee around 210 GPa, not supporting the interpretation as a polymorphic transition. Furthermore, the obtained Mo Hugoniot and sound velocity data are compared with the results calculated using QEOS model.

10:30AM H2.00005 No solid-solid phase transition in Mo before melting: experiment and theory1, XIULU ZHANG, Laboratory for Shock Wave and Detonation Physics Research, IFP, CAEP, ZHONGLI LIU, College of Physics and Electric Information, LYNU, KE JIN, FENG XI, YUYING YU, YE TAN, CHENGDA DAI, LINGCANG CAI, Laboratory for Shock Wave and Detonation Physics Research, IFP, CAEP — Whether there is a solid-solid phase transition plays an important role in shaping the phase diagram of Mo. Previous sound velocity measurements suggested one at 210 GPa[Phys. Rev. Lett. 62, 637(1989)], but the latest results [J. Nguyen, et al., In Shock Compression of Condensed Matter-2011] did not support it. In our work, adopting the “reverse impact” method[J. Geophys. Res. 100(B1), 529 (1995)] and the “overtake” method[Rev. Sci. Instrum. 53, 245(1982)], we obtained new data in the pressure range from 160 GPa to 160 GPa. Together with the latest results, it can be concluded that a solid-solid phase transition does not occur in Mo under shock loading pressures from 38 GPa to 240 GPa. With the crystal structure prediction techniques based on the genetic algorithms and density functional theory calculations, two metastable structures C2m and I4mmm are found, but we did not reproduce fcc phase of Mo in our searches. As their energy is much higher than that of bcc Mo, it is unlikely that they are more stable than bcc Mo at high temperatures. This is consistent with C. Cazorla’s conclusion that fcc is less stable than bcc[Phys. Rev. B 85, 064113(2012)], and theoretically support the conclusion of our sound velocity measurements.

1Supported by NSAF under Grant Nos. U1230201and 10776029, NSF under Grant Nos. 11104227, and 11104127, the project 2010A0101001 by CAEP, the Defense Industrial Development Program under Grant No. B1520110001, and the project 11zxj04 from LECMP of SWUST.

Tuesday, July 9, 2013 9:15AM - 10:45AM –
Session H3 NT.1 Novel Techniques: PDV
Fifth Avenue - David Chapman, Imperial College London

9:15AM H3.00001 Comprehensive Comparison of VISAR and PDV Laser Interferometry in Plane Shock Wave Experiments, K.A. ZIMMERMAN, Washington State University, A.J. IVERSON, E.P. DAYKIN, National Security Technologies, LLC, Y. TOYODA, Washington State University, G.D. STEVENS, R.S. HIXSON, National Security Technologies, LLC, Y.M. GUPTA, Washington State University — Plate impact experiments, using well-characterized materials, were conducted to achieve a direct and comprehensive comparison of two laser interferometry approaches used to measure shock wave profiles: Velocity Interferometer System for Any Reflector (VISAR) and Photon Doppler Velocimetry (PDV). A unique feature of this study was a one-to-one comparison of the two measurement approaches in each experiment. A broad range of stresses (4-60 GPa) were examined in this study. The choice of impactor and target materials permitted us to examine different types of material responses (elastic, elastic-plastic, and time-dependent elastic-plastic deformation) which, in turn, resulted in different types of wave profiles (single wave, two-wave structure, and two-wave structure with rapid stress relaxation following the first wave). Overall, the two approaches showed good agreement. However, small but discernible differences were observed in the following situations: wave profiles involving rapid stress relaxation behind the elastic wave; and window-corrected, peak states at high stress. The relative strengths and weaknesses of both methods are summarized. Work supported by DOE/NNSA.

9:30AM H3.00002 PDV experiments on size-calibrated particles accelerated using a pulsed laser, PATRICK MERCIER, GABRIEL PRUDHOMME, CEA, DAM,DIF, LAURENT BERTHE, PIMM, UMR 8006 CNRS-Arts et Métiers ParisTech, 151 bd de l'Hôpital, F-75013 Paris, JACKY BENIER, PIERRE-ANTOINE FRUGIER, CEA,DAM,DIF — In order to observe a particle cloud produced at the output face of a shock-loaded plate, we performed several experiments with size-calibrated particles deposited on an Aluminum plate. It was shock-loaded using a pulsed laser (1 J, 10 ns, 532 nm) resulting in an acceleration of the particles up to 100 m/s. Various experiments have been performed to study the influence of different parameters: the particle material (Cu, Al, Au), the particle diameter (a few micrometers), the thickness of the deposited particle layer and the shock pressure. We recorded the back-reflected light with both orthogonal and tilted probes, and we present the corresponding PDV spectograms displaying cloud velocities as well as velocity tracks due to individual particles. Some of them decelerate within the ambient gas while others, non-spherical, also rotate. By applying a deceleration model, we were able to determine the initial particle velocities and their sizes. The obtained sizes are consistent with the manufacturer values. In addition, the tilted probes could be used to infer information on the shape of the moving particle clouds.
9:45 AM H3.00003 New developments in PDV. Erik Moro, Los Alamos National Laboratory — Photon Doppler velocimetry (PDV) has made the transition among many experimental groups from being a new diagnostic to being routinely fielded as a means of obtaining velocity data in high-speed test applications. Indeed, research groups both within and outside of the shock physics community have taken note of PDV's robust, high-performance measurement capabilities. As PDV serves as the primary diagnostic in an increasing number of experiments, it will continue to find new applications and enable the measurement of previously un-measurable phenomena. This paper provides a survey of recent developments in PDV system design and feature extraction as well as a discussion of new advances for PDV. Specifically, changes at the system level have enabled the collection of data sets that are far richer than those previously attainable in terms of spatial and temporal coverage as well as improvements over PDV's previously measurable velocity ranges. And until recently, PDV data have been analyzed almost exclusively in the frequency-domain; although the use of additional data analysis techniques is beginning to show promise, particularly as it pertains to extracting information from a PDV signal about surface motion that is not along the beam’s axis.

10:15 AM H3.00004 PDV experiments on shock-loaded particles. Gabriel Prudhomme, Patrick Mercier, CEA, DAM, DIF, Laurent Berthe, PIMM, UMR 8006 CNRS-Arts et Metiers ParisTech, 151 bd de l'Hôpital, F-75013 Paris, DAVINA SIHACHAKR, CHRISTIAN RION, CEA, DAM, DIF — We present results from PDV experiments in which particles are ejected from shock-loaded metallic plates. The shocks in these samples were generated using either a pulsed laser or high-explosive plane-wave generators. In a first series of experiments, we deposited size-calibrated particles (around 10-μm in diameter) on the target surface. We visualized the back-reflected light to infer the free surface and particle velocities (up to several km/s), as well as the cloud structure, as a function of the variable parameters: the particle material (tin, copper, gold, etc.), the particle diameters (a few microns) and the thicknesses of the deposited particle layer. In the second series of experiments, we observed the particles created by microjetting, microspalling or melting at the free surface of tin plates. The slowing down of the particles in air has been measured and, in some experiments, the interaction of secondary shockwave with the particle cloud has also been observed. Finally, we compare these results to those obtained with simple models and with a hydrodynamic code (Hésione).

10:30 AM H3.00005 3D Hemispherical Test Development to Evaluate Detonation Wave Breakout. Elizabeth Francois, John Morris, Mark Lieber, Larry Hill, Los Alamos National Lab — The onionskin test has been the standard test to evaluate detonation wave breakout over a hemispherical surface for decades. It is not without its shortfalls however. It only images a small portion of the explosive and requires very precise alignment and camera requirements to make sense of the results. Asymmetry in explosive behavior cannot be pinpointed or evaluated effectively. We have developed a new diagnostic using fiber optics covering the surface of the explosive to yield a 3D representation of the detonation wave behavior. Precise timing mapping of the detonation over the hemispherical surface is generated which can be converted to detonation wave breakout behavior using Hugoniot's wave reconstruction. This presentation and paper will include the results of a recent suite of tests. The results of these tests will describe the effects on detonation wave breakout symmetry when inert materials are placed between the detonator and booster. The value of this test in visual representation of dynamic behavior will be presented and discussed. Statistical analysis of the test as compared to the onionskin test will be outlined. Test limitations and future improvements will be discussed.

Tuesday, July 9, 2013 9:15AM - 10:45AM — Session H4 TM First Principles Methods III
Vashon - Ann Mattsson, Sandia National Laboratories

9:15 AM H4.00001 Merging Kohn-Sham and Orbital-Free DFT Calculations to Extend the LiH Hugoniot to Very High Pressures. Joel D. Kress, Los Alamos National Laboratory — Large-scale hydrodynamic simulations of fluids and plasmas under extreme conditions require knowledge of various properties such as the equation of state (EOS), mass diffusion, and shear viscosity. While many approaches exist for the determination of these properties, one of the most accurate employs quantum molecular dynamics (QMD) simulations on large samples of atoms of the various species. Examples include the shock compression of metal hydrides and the mixing of deuterium/tritium (DT) fuel with lithium hydride (LiH). This work is part of an ongoing collaboration with L. A. Collins, S. Crockett, M. P. Desjarlais, and F. Lambert and under the auspices of an agreement between CEA/DAM and NNSA/DP on test limitations and future improvements will be discussed.

9:45 AM H4.00002 First-principles entropy calculations for liquid metals and warm dense matter. Michael Desjarlais, Sandia National Laboratories, Albuquerque, New Mexico — The total entropy is not an explicit or easily accessible quantity in first-principles molecular dynamics simulations. It is, however, an extremely important quantity for the calculation of total free energies and derived properties such as equilibrium phase boundaries. In shock experiments the entropy of the shock state determines the release isentrope. Recent advances in the calculation of the entropy for liquid metals and warm dense matter directly from the velocity history in quantum molecular dynamics simulations are presented. The method, a generalization of the 2PT method for classical molecular dynamics [Lin, et al., J. Chem. Phys. 2003], significantly increases the accuracy of the method for systems with electronic entropy, spin degrees of freedom, and the softer interactions characteristic of liquid metals and warm dense matter. The results are compared to data and the results of indirect methods, such as coexistence simulations to determine phase boundaries.

4:30 PM H5 ABSTRACT WITHDRAWN

10:00 AM H4.00003 Density Functional Theory Investigation of Sodium Azide at High Pressure. Brad Steele, Aaron Landerville, Ivan Oleynik, University of South Florida — Sodium azide is being investigated as a potential precursor to a high-nitrogen content energetic material. Changes in the experimentally measured raman spectra under compression and high temperature indicate that a structural change may have taken place. Accurate mode assignments of new peaks arising in the raman spectra have been inconclusive. In this work, the first order rama spectra of sodium azide’s alpha and beta phases are calculated using Density Function Perturbation Theory (DFPT) under compression and expansion. Normal mode assignments are made and compared to experiment. In addition, the equation of state of both phases is obtained up to 90 GPa.

10:15 AM H4.00004 ABSTRACT WITHDRAWN
Tuesday, July 9, 2013 9:15AM - 10:45AM –
Session H5 GP1: Geophysics II

Cascade I - Natalia Dubrovinskaia, University of Bayreuth

10:30AM H4.00005 Finite temperature orbital-free density functional theory MD for warm dense matter systems

TRAVIS SJOSTROM, JEROME DALIGAULT, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Warm dense systems present significant challenges for ab initio simulations. In order to incorporate the quantum nature of these systems, state of the art approaches use Kohn-Sham DFT. The number of orbitals required in this approach however scales with the temperature, making it computationally prohibitive. In recent years attention has been given to orbital-free (OF) DFT, which depends only on the density and does not suffer the same scaling issue. For the most part the finite temperature Thomas-Fermi approximation has been used, with some efforts making use of the gradient expansion, or a generalized gradient form. Interestingly, zero temperature OF DFT efforts have made use of non-local functionals based upon linear response theory, with marked improvement over gradient methods. Here we explore extension of this approach to finite temperature. We have implemented the new approximations in both an average atom scheme and for extended systems in OF MD, and will present here the results for system in the warm dense matter regime.

1 Work supported by the NNSA of the U.S. DOE at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

Tuesday, July 9, 2013 9:15AM - 10:45AM –
Session H5 GP1: Geophysics II

Cascade I - Natalia Dubrovinskaia, University of Bayreuth

9:15AM H5.00001 Analytic multiphase equation of state for MgO

O. HEUZE, Commissariat a l’Energie Atomique, D.C. SWIFT, Lawrence Livermore National Laboratory, N.D. DRUMMOND, University of Lancaster, R.G. KRAUS, Harvard University, G.J. ACKLAND, University of Edinburgh — MgO is an important prototype and end-member constituent for the mantle of rocky planets. Planetary structures and the response to impacts depend on the equation of state (EOS), notably including any phase transitions. MgO adopts the B1 crystal structure under ambient conditions, and has been predicted to change to B2 under compression. There are large variations in theoretical predictions of this transition and of the conditions for shock melting; experimental observations are inconsistent or unclear. We have previously constructed equilibrium B1-B2 EOS for MgO, in tabular form, using ab initio electronic structure calculations based on density functional theory and the quasiharmonic approximation for lattice vibrations. Here, we use our new formalism for thermodynamically-complete Mie-Grüneisen EOS to construct an analytic, multiphase EOS for MgO. We also constructed an approximate liquid EOS as a perturbation of the B1. We investigated the effect of phase change kinetics, including an asymptotic case in which the Maxwell construction is omitted. The principal shock Hugoniot calculated using kinetics appears to agree closely with pressure-temperature states measured for a decaying shock, corresponding to the B1-B2 region of the EOS.

9:30AM H5.00002 Elastic Anisotropy and Auxetic Behavior in Minerals

THOMAS DUFFY, Princeton University — The elastic properties of minerals are of fundamental importance for understanding thermodynamic and mechanical behavior as well as for interpretation of seismic data. In recent years, there has been renewed interest in novel aspects of single-crystal elastic behavior. A database of single-crystal elastic properties of minerals and related phases has been constructed in order to evaluate auxetic behavior among minerals at ambient conditions and at high P and T. Partially auxetic behavior (directions with negative Poisson’s ratios) is common among minerals, especially among the quartz, rutile, calcite, spinel, and sapphireite structures. Auxetic behavior is most common in the cubic and trigonal systems and correlates strongly with the elastic anisotropy as measured by the universal anisotropy index. MgO provides a striking example of P-T tuning of auxeticity and anisotropy. The larger variation in elastic anisotropy of MgO from ambient P and 3000 K to ambient T and 250 GPa samples nearly the entire range of extrema in Poisson’s ratio of cubic crystals. MgO is strongly auxetic along [110] at high temperatures.

9:45AM H5.00003 MgO melting curve constraints from shock temperature and rarefaction overtake measurements in samples preheated to 2300 K

O.V. FAT’YANOV, P.D. ASIMOW, Division of Geological and Planetary Sciences, Caltech, Pasadena, CA 91125 U.S.A. — In a continuous effort to determine experimentally the melting curve of MgO at 100-200 GPa, we extended our target preheating capability to 2300 K. The limit was primarily caused by intense sublimation of pure MgO in vacuum above 2050 K. Completely redesigned Mo capsules holding ~20 mm long MgO crystals with controlled thermal gradients were impacted by thin Ta flyers launched at 6.5 to 7.5 km/s on the Caltech two-stage light-gas gun. Radiative shock temperatures and rarefaction overtake times were measured simultaneously by a 6-channel pyrometer with 3 ns time resolution, over 440-750 nm spectral range. All our experiments showed smooth pressure dependence of MgO sound speed consistent with the solid phase at 204-239 GPa. Observed temperatures are ~1000 K lower than those predicted by the solid phase model, but the plot of measured shock temperature versus pressure exhibits a pattern typical of shock melting at the highest pressure investigated. This may suggest that the Hugoniot of MgO preheated to 2300 K crosses its melting line at 220-240 GPa. Sound speed data indistinguishable from the solid phase model do not exclude the possibility of melting there.

10:00AM H5.00004 Ramp compression of magnesium oxide to 234 GPa

JUE WANG, Princeton University, RAYMOND F. SMITH, FEDERICA COPPARI, JON H. EGGERT, LLNL, THOMAS R. BOEHLY, LLE, GILBERT W. COLLINS, LLNL, THOMAS S. DUFFY, Princeton University — Periclase, MgO, is of fundamental importance for geophysics as the end-member of the ferropericlase, (Mg,Fe)O, solid solution. It is also of interest for understanding the interiors of extrasolar planets. In this work, we report a study of MgO using laser-based ramp compression. Ramp wave loading can be used to obtain equation-of-state data in the region of thermodynamic space lying between the principal isentrope and Hugoniot. Ramp compression experiments were performed using the Omega laser at LLE of the University of Rochester. A series of three steps were lithographically etched into a single-crystal MgO wafer that was then polished to the requisite thickness. A planar compressive wave was launched into the sample with high-powered ramp-shaped laser pulse. The free surface velocities of different sample thicknesses were measured using a line-imaging VISAR. The velocity profiles were integrated to obtain the stress-density response using a Lagrangian analysis technique. Our experiments reached a maximum pressure of 234 GPa, and the measured equation of state is consistent with previous shock and static studies.

1 The research was supported by NNSA/DOE through the National Laser Users’ Facility Program under contracts DE-NA0000856 and DE-FG52-09NA29037.

10:15AM H5.00005 Transport properties of the Earth’s core

DARIO ALFE, University College London — I will report on the thermal and electrical conductivities of iron and two liquid silicon-oxygen-iron mixtures (Fe0.82Si0.10O0.08 and Fe0.70Si0.09O0.13), representative of the composition of the Earth’s outer core at the relevant pressure-temperature conditions, obtained from density functional theory calculations with the Kubo-Greenwood formulation. We find thermal conductivities $k = 100 (160)$ W m$^-1$ K$^-1$, and electrical conductivities $\sigma = 1.1 (1.3) \times 10^9$ S m$^-1$ at the top (bottom) of the outer core. These values are between 2 and 3 times higher than previous estimates, and have important implications for our understanding of the Earth’s thermal history and the functioning of the Earth’s magnetic field, including rapid cooling rate for the whole core or high level of radiogenic elements in the core.

Tuesday, July 9, 2013 9:15AM - 10:45AM –
Session H6 EM.1 Ignition I

Cascade II - Michael Hobbs, Sandia National Laboratories
Mechanical Fluctuations and Microstructure

There remains great interest in predicting the response of energetic materials to impact stimulus from a performance standpoint. In most conventional condensed-phase energetic materials, this response is governed by characteristics of the microstructure below the macroscale. To better understand the response of energetic materials to impact, a mesoscale model has been developed. The objective of this work is to show the capability of modeling the response of heterogeneous energetic materials without relying on data fitting routines, and to use these models to investigate the physics of shock response and how they lead to shock to detonation transition. To this end, a first principles model was used to parameterize a variable heat capacity Mie-Gruneisen model for the condensed phase EOS. Using the realistic hot-spot states made possible by this EOS, trends from the historical parameter space of flyer impact experiments were reproduced. These results highlight the importance of the EOS in grain-scale reactive burn models, and showcase the predictive capabilities of these models when coupled with a valid unreacted EOS.

Thermomechanical Response of HMX Polycrystals to Simulated Impact Loading

A framework for analyzing the thermo-mechanical response of ensembles of HMX crystals to impact loading is presented. The effects of material microstructure and anisotropy on heating and stress evolution are investigated. The model accounts for anisotropic elasticity, crystalline plasticity, and thermal conduction. Simulations carried out concern the response of full dense HMX polycrystalline ensembles under loading at impact velocities from 50 - 400 m/s. Herein, the effect of the inherent anisotropies on the energy and stress localization in an HMX based PBX is quantified. The results show that when local stress and temperature states are critical, such as energetic composites, modeling the crystalline anisotropy of the constituents is essential to capturing the whole range of states experienced by the material.

Microstructural Effects on the Ignition Behavior of Various HMX Materials

The detonation physics community has embraced the idea that initiation of high explosives proceeds from an ignition event through subsequent growth to steady detonation. This construct is the basis for the well-known Lee-Tarver reactive flow model. A weakness of all the commonly used ignition and growth models is that microstructural characteristics are not explicitly incorporated in their ignition terms. This is the case in spite of a demonstrated, but not well-understood, empirical link between morphology and initiation of energetic materials. Morphological effects have been parametrically studied in many ways, with the majority of efforts focused on establishing a tie between bulk powder metrics and ignition of the consolidated material. More recently, there has been a shift toward characterizing the microstructure of consolidated materials in order to understand the underlying mechanisms governing performance. We have assessed the utility of using the James’ Ignition model as a tool to quantify effects of bed microstructure on ignition behavior. We have studied the ignition behavior of four types of HMX materials ranging from fine particle fluid energy milled to coarse particle material. We will also report characterization of the pressed microstructure of each of the various materials and discuss how the measured ignition behavior may have been influenced.

Dissipative Heating in Porous Solid Explosives: Correlation of Thermomechanical Fluctuations and Microstructure

Materials having similar effective (or average) porosities and composition, and particle size and shape distributions, may have different impact responses due to spatial fluctuations in these quantities at the particle scale. In this study, a combined finite and discrete element technique is used to computationally examine the inert impact response of aluminized HMX for different effective porosities and metal mass fractions, and explosive and metal particle sizes. Emphasis is placed on examining the statistical correlation between predicted fluctuations in thermo-mechanical fields within and behind compaction waves and the local microstructure. To this end, predicted fields are mapped onto the initial material configuration and analyzed using multivariate Principal Component Analysis (PCA). Preliminary predictions will be given that identify microstructural features, or combinations of features, that result in a high probability of hot-spot formation and their dependence on impact speed.

H6.00003 Mesoscale Simulations of Reaction Initiation and Growth in HE Composites using PBRB model

Two-dimensional (2D) finite element based mesoscale simulation results are presented to predict reaction initiation and growth in high energy (HE) composites using the physics based reactive urn (PBRB) model. The HE composites are modeled as an ensemble of grains with statistically-distributed second phase particles. Their shock response is modeled with elastic-inelastic deformation coupled with the PBRB equation-of-state model. The inter-grain response is described by the contact-cohesive model that allows grain boundary failure and creation of free surface with friction characteristics during compressive shock loading. The heat generation due to the non-linear elastic, inelastic, cohesive, and friction energy dissipation into pre-assumed statistically-distributed hot spots, surface sublimation, and gas phase reaction are described as coupled mechanisms by the PBRB model yielding the mean stress as a function of the reaction at any given time. The simulations predict the time and run to detonation with reasonable agreement with data. The relative merits of 1D hot spot idealization, embodied in the PBRB model, for generic mesoscale simulations will be discussed.

H6.00004 Thermomechanical Response of HMX Polycrystals to Simulated Impact Loading

A framework for analyzing the thermo-mechanical response of ensembles of HMX crystals to impact loading is presented. The effects of material microstructure and anisotropy on heating and stress evolution are investigated. The model accounts for anisotropic elasticity, crystalline plasticity, and thermal conduction. Simulations carried out concern the response of full dense HMX polycrystalline ensembles under loading at impact velocities from 50 - 400 m/s. Herein, the effect of the inherent anisotropies on the energy and stress localization in an HMX based PBX is quantified. The results show that when local stress and temperature states are critical, such as energetic composites, modeling the crystalline anisotropy of the constituents is essential to capturing the whole range of states experienced by the material.

Session H7 CH.1 Chemistry: High Pressure Synthesis

Tuesday, July 9, 2013 9:15AM - 10:45AM

9:15AM H6.00001 Dissipative Heating in Porous Solid Explosives: Correlation of Thermomechanical Fluctuations and Microstructure

9:30AM H6.00002 HNS EOS Refinements and Qualitative Experimental Parameter Space Modeling

10:00AM H6.00004 Thermomechanical Response of HMX Polycrystals to Simulated Impact Loading

10:15AM H6.00005 Microstructural Effects on the Ignition Behavior of Various HMX Materials
Theoretical predictions for superior material properties, such as ultra-hardness, superior transport properties such as electrical and thermal conductivity, high energy-density, high-temperature superconductivity, ability to storage hydrogen, etc. Synthesis of new materials at high pressures is based on changes in the equilibrium chemical bonding. Moreover, materials with “unusual” stoichiometries have been predicted to become thermodynamically stable at high pressures. Implications of this novel extreme chemistry for synthesis of new materials for practical applications remain challenging because high-pressure bonding patterns are often thermodynamically unstable at ambient pressure. Search for a recovery mechanisms or attempts of synthesis in nominally metastable conditions require detailed knowledge of the energy landscape; extensive collaborative efforts of experiment and theory are needed for its determination. Here, I emphasize the importance for this task of in situ fast diagnostic methods. I will present new results on synthesis of materials with new bonding patterns and unusual stoichiometries containing hydrogen, nitrogen, carbon, and halogens. This work has been performed in collaboration with M. Somayazulu, V. V. Struzhkin, V. Prakapenka, E. Stavrou, T. Muramatsu, M. Antipov, V. Igonin, A. Lebedev, M. Rauschenbach, A. Sadunov, A. Utenkov, A. N. Carrara, IFAC-CNR — Mesos/micro-porous solids such as zeolites are complex materials exhibiting an impressive range of applications, including molecular sieve, gas storage, catalysis, electronics and photonics. We used these materials, particularly non-catalytic zeolites in an entirely different fashion. In fact, we performed high pressure (0.5-30 GPa) chemical reactions of simple molecules on a sub-nanometer scale in the channels of a pure SiO$_2$ zeolite, silicalite to obtain unique nano-composite materials with drastically modified physical and chemical properties. Our material investigations are based on a combination of X-ray diffraction and optical spectroscopy techniques in the diamond anvil cell. We will first briefly show how silicalite can be easily filled by simple molecules such as Ar, CO$_2$ and CH$_4$ among others from the fluid phase at high pressures, and how this efficient filling removes the well known pressure induced amorphization of the silica framework (Haines et al., JACS 2010). We will then present on a silicon carbonate crystalline phase synthesized by reacting silicate and molecular CO$_2$ that fills the nano-pores, at 18-26 GPa and 600-980 K; after the synthesis the compound is temperature quenched and it results to be slightly metastable at room conditions (Santoro et al., PNAS 2011). On the other hand, a stable at room condition spectacular crystalline nano-composite is obtained by photo-polymerizing ethylene at 0.5-1.5 GPa under UV (351-364 nm) irradiation in the channels of silicalite (Santors et al., Nat. Commun., in press 2013). For this composite we obtained a structure with single polyethylene chains adapting very well to the confining channels, which results in significant increases in bulk modulus and density, and the thermal expansion coefficient changes sign from negative to positive with respect to the original silicate host. Mechanical properties may thus be tuned by varying the amount of polymerized ethylene. We then think our findings could allow the high pressure, fast catalysis of a unique generation of technologically, functional materials based on simple hydrocarbons polymerized in conforming meso/micro-porous solids.

Growth of rectangular hollow tube single crystals with rutile-type structure in supercritical fluids, KEN NIWA, TOMOHARU TUKUNAGA, MASASHI HASEGAWA, Nagoya University — Super critical fluid is known as a suitable solvent in the dissolution and extraction process, due to its extreme high solubility and reactivity. On the other hand, further experimental approaches using supercritical fluid would offer new insights, especially in the field of novel material synthesis and crystal growth. We here report on the successful growth of single crystals with the rutile-type structure (3/10$_2$ : $M$ = Ti, Si, Ge and Sn) in the supercritical fluids (water or oxygen) by using laser heated diamond-anvil cell at above 5 GPa. The resultant product showed the rectangular hollow tube with several tens of microns in length and the wall thickness of less than 500 nm. TEM analyses demonstrated that this rectangular hollow tube single crystal is surrounded by the (110) face and grown along the [001] direction. The preferential growth of (110) face is consistent with the lowest surface energy of (110) in the rutile-type structure. In addition, the rapid cooling rate of LHDA and the high-solubility of oxides into the supercritical fluids also play an important role for the formation of the rectangular hollow tube. The details of the experiments will be discussed in the presentation.

High-pressure synthesis of new materials via formation of new bonding patterns and unusual stoichiometries, ALEXANDER GONCHAROV, Geophysical Lanboratory, Carnegie Institution of Washington — The search for new materials synthesized under extreme conditions of high pressure and high pressure is currently actively pursued. There are multiple theoretical predictions for superior material properties, such as ultra-hardness, superior transport properties such as electrical and thermal conductivity, high energy-density, high-temperature superconductivity, ability to storage hydrogen, etc. Synthesis of new materials at high pressures is based on changes in the equilibrium chemical bonding. Moreover, materials with “unusual” stoichiometries have been predicted to become thermodynamically stable at high pressures. Implications of this novel extreme chemistry for synthesis of new materials for practical applications remain challenging because high-pressure bonding patterns are often thermodynamically unstable at ambient pressure. Search for a recovery mechanisms or attempts of synthesis in nominally metastable conditions require detailed knowledge of the energy landscape; extensive collaborative efforts of experiment and theory are needed for its determination. Here, I emphasize the importance for this task of in situ fast diagnostic methods. I will present new results on synthesis of materials with new bonding patterns and unusual stoichiometries containing hydrogen, nitrogen, carbon, and halogens. This work has been performed in collaboration with M. Somayazulu, V. V. Struzhkin, V. Prakapenka, E. Stavrou, T. Muramatsu, A. Oganov, W. Zhang, Q. Zhu, S. E. Boullie, A. O. Lyakhov, Z. Konopkova, H.-P. Liermann, D.-Y. Kim.

The model of particle ejection from a metal free surface, ALLA GEORIEVSAYA, MICHAEL ANTIPOV, VLADISLAV IGININ, ALEXANDER LEBEDEV, MARGARITA LEBEDEVA, KONSTANTIN PANOV, VADIM KNYAZEV, VICTOR RASMUSKY, VALEMY SADUNOV, ALEXANDER UTENKOV, RFNC-VNIIEF — We present theoretical and computational results of ejecta investigations. We have developed a new model of ejecta taking into account the influence of a shock wave profile on areal mass (unit area) of ejected particles, a temporal and spatial particle density distribution. According to our analytic solution when the metal free surface interacts with the Taylor wave the mass of ejected particles have developed a new model of ejecta taking into account the influence of a shock wave profile on areal mass (unit area) of ejected particles, a temporal and spatial particle density distribution. According to our analytic solution when the metal free surface interacts with the Taylor wave the mass of ejected particles is less than in case of interaction of the free surface with a supported shock wave. Furthermore, according to this model the total mass of ejecta is independent of shock wave pressure but depends on a correlation of initial perturbations on the free surface and a shock wave pulse duration $\Delta x$, i.e. $m_e = f(k^2 - a^2 \cdot \Delta x)$, where $a_0$ — a perturbation amplitude, $k = 2\pi/\lambda$ — a mode number, $\lambda$ — a perturbation wavelenght. The model also determines the ejecta time which depends on the metal free surface velocity, the shock wave pulse duration and the initial perturbations. This solution is applied to metals when the strength does not affect the Richtmyer-Meshkov instability. We evaluated the total mass of ejected particles and particle density distribution. These estimates conform to the experimental results.
11:15AM J1.00002 Using High Energy Diffraction Microscopy to Assess a Model for Microstructural Sensitivity in Spall Response\textsuperscript{1}

NATHAN BARTON, JOEL BERNIER, MOON RHEE, SHIU FAI LI, MUKUL KUMAR, Lawrence Livermore National Laboratory, JOHN BINGERT, Los Alamos National Laboratory, JONATHAN LIND, Carnegie Mellon University — We present results from a model validation effort that employs detailed non-destructive three-dimensional microstructure data obtained from High Energy Diffraction Microscopy (HEDM) experiments. By focusing validation efforts on models that connect directly to experimentally measurable features of the microstructure, we can then build confidence in the use of models for components prepared under different processing routes, with different impurity distributions, or subjected to different loading conditions. The computational model makes use of a crystal mechanics based constitutive model that includes porosity evolution. The formulation includes nucleation behavior that is fully integrated into a robust numerical procedure, enhancing capabilities for modeling small length scales at which nucleation site potency and volume fraction are more variable. Three-dimensional experimental data are available both pre-shot and post-shot from the same volume of impact-loaded copper. Crystal lattice orientation and porosity data are obtained, respectively, from near-field HEDM and tomography techniques. Starting from the as-measured initial microstructure, simulation results will be compared to post-shot experimental results as a function of modeling assumptions.

\textsuperscript{1}This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

11:30AM J1.00003 Fragmentation Under Extreme Conditions: Applications to Risk Assessment and Diagnostic Development at Mega-Joule Class Laser Facilities

JAMES STOLKEN, Lawrence Livermore National Laboratory — The development of Mega-Joule class laser facilities (NIF, USA; LMJ, France, SG-IV, China) has driven the need to understand, predict, and control the risks associated with experimental operations due to ablation, blast, and impact hazards. These hazards potentially jeopardize a broad range of facility assets, such as Targets, Laser Optics, Diagnostics, and other Infrastructure. This presentation shall focus on the application of high-performance computer modeling and simulation (M&S) to quantify and mitigate the risk posed by blast, ablation, and impact hazards. The overall risk management strategy is discussed and the role of M&S outlined. The M&S activities fall within two broad categories, Laser-Material interaction (LM) and Hydro-Structural (HS) simulations. The LM class of simulations addresses the high energy, short time phenomena including laser energy deposition, radiation, ablation, heat-flow, and hydrodynamic motion. The HS class of simulations addresses lower energy, longer time phenomena including hydrodynamic motion, heat-flow, material failure, fracture, and fragmentation. Recent efforts to assess and improve fragmentation simulation capabilities are reviewed. Existing simulations methodologies are evaluated and compared to high fidelity fragment data. Applications to diagnostic development and experimental design are reviewed.

In collaboration with Nathan Masters, Aaron Fisher, Brian Pudliner, Mukul Kumar, Matthew Barham, and Cal Smith, Lawrence Livermore National Laboratory.

12:00PM J1.00004 Surface nano-structuring produced by spallation of metal irradiated by ultrashort laser pulse

NAIL INOGAMOV, Landau Institute for Theoretical Physics of RAS, VASILY ZHAKHOVSKY, YUSUF EMIROV, IVAN OLEYNIK, University of South Florida, SERGEY ASHITKOV, MIKHAIL AGRANAT, ANATOLY FAENOV, Joint Institute for High Temperatures of RAS, TATIANA PIKUZ, MASAHIKO ISHINO, NOBORY HASEGAWA, MASAHIKO KASAHARA, Physics Beam Science Directorate, JAEA — Response of metal to heating by ultrashort laser pulse was studied using both two-temperature hydrodynamics modeling and molecular dynamics simulation. Our simulations of Al, Ni and Ta showed that deposition of laser energy in range of ~ 50-200 mJ/cm\textsuperscript{2} in a thin surface layer leads to high electron temperature, which propagates supersonically into the bulk of metal. As a result, the thicker heated layer of ~ 100 nm deep with molten metal in electron-ion thermal equilibrium is formed after several picoseconds. Because expansion of the layer into vacuum, the tensile wave propagates into metal and may produces significant negative pressure. Above some critical energy deposition where the tensile stress exceeding the strength of liquid metal, many voids start to nucleate beneath the surface forming a foam-like material, which may lead to spallation of a liquid shell if its kinetic energy is enough to overcome the tensile strength of foam. We found that the fluence threshold for cavitation is about a few tens percent less than the spallation threshold. Simulated evolution of surface liquid foam, including its breakings and freezing with formation of 3-D nanostructures on surface, was compared with our experimental observations.

12:15PM J1.00005 Ejecta size distribution from the dynamic fragmentation of shock-loaded Cu and Sn metals under melt conditions

OLIVIER DURAND, LAURENT SOULARD, CEA, DAM, DIF, F-91297 Arpajon, France — Large scale molecular dynamics (MD) simulations are performed to study and to model the ejecta production from the dynamic fragmentation of shock-loaded metals under melt conditions. A generic 3D crystal with about 10\textsuperscript{8} atoms in contact with vacuum and with a sinusoidal free surface roughness is shock loaded above its fusion point. Two metals are studied (Cu and Sn) and the amplitude of the roughness is varied. The simulations show that the associated time resolved ejecta mass (or size) distributions exhibit a generic behavior with the sum of two distinct terms: in the small size limit, the distribution obeys a power law dependence and in the large size limit, it obeys an exponential form. With the help of additional simple simulations, we show that these two components are the signature of two distinct basic mechanisms of fragmentation. The power law dependence results from the fragmentation of a 2D fractal network of ligaments of liquid metals generated during the ejection process. The exponential distribution results from a 1D Poisson fragmentation mechanism of the largest ligaments previously generated.

Tuesday, July 9, 2013 11:00AM - 12:30PM — Session J2 CM.4 Warm Dense Matter I — Grand Ballroom II - Damian Swift, Lawrence Livermore National Laboratory

11:00AM J2.00001 Two-temperature hydrodynamics of laser-generated ultrashort shock waves in elasto-plastic solids

DENIS ILNITSKY, All-Russia Research Institute of Automatics, VIKTOR KHOKHLOV, NAIL INOGAMOV, YURI PETROV, Landau Institute for Theoretical Physics of RAS, VASILY ZHAKHOVSKY, University of South Florida, KIRILL MIGDAL, All-Russia Research Institute of Automatics, SERGEY ANISIMOVA, Landau Institute for Theoretical Physics of RAS — Femtosecond laser is a unique tool for generation of ultrashort laser pulse. Results of 2T-HD simulation of plastic and super-elastic shock wave propagation in Al and Ni at later stage is in good agreement with that in splitting two-wave regime the elastic precursor can have longitudinal stress nearly 30 times as large as the conventional Hugoniot elastic limit. To generate very high deformation rates in target materials. It was recently found in experiment [1] and molecular dynamics (MD) simulation [2] that nucleation behavior can have longitudinal stress nearly 30 times as large as the conventional Hugoniot elastic limit. To generate very high deformation rates in target materials. It was recently found in experiment [1] and molecular dynamics (MD) simulation [2] that nucleation behavior can have longitudinal stress nearly 30 times as large as the conventional Hugoniot elastic limit.

\textsuperscript{1}S. I. Ashitkov, M. B. Agranat, G. I. Kanel’, et al, JETP Letters, 92, 516 (2010)
\textsuperscript{2}V. V. Zhakhovskii and N.A. Inogamov, JETP Letters, 92, 521 (2010)
11:15AM J2.00002 Crystal-like and plasma-like properties of the two-temperature WDM. VLADIMIR STEGAILOV, GENRI NORMAN, SERGEY STARIKOV. Joint Institute for High Temperatures RAS — The two-temperature warm dense matter (WDM) is produced for short times at the interaction of fs and ps laser radiation with solid surfaces, propagation of a fast ion through condensed matter and at some other advanced experiments. The theory of such transient nonequilibrium WDM states is a challenging problem since electron temperature is about several eV, but ions remain to be cold and keep original crystallographic positions for several ps. Therefore the band structure survives but electron and phonon energy dispersions are changed due to the inverse influence of the electron excitation. Ion cores survive as well but their inner shells are partially excited and their populations follow plasma behavior. So the temporary WDM states considered demonstrate both crystal and plasma features like a crystal-plasma “centaur.”

The methods of molecular dynamics and collisional-radiative kinetics are used to investigate the plasma properties of WDM. The transient but quasi-stationary for a short time state of non-equilibrium, uniform electron plasmas can be both strongly and weakly coupled. X-ray spectral lines are emitted by ion cores embedded in electron plasma environment which influences the spectra strongly.

11:30AM J2.00003 Equation of state measurement of shock-released carbon. KATERINA FALK, JOHN F. BENAGE, ROBERT G. WATT, DAVID S. MONTGOMERY, JAMES R. WILLIAMS, DEREK W. SCHMIDT, Los Alamos National Laboratory, ELISEO J. GAMBOA, PAUL A. KEITER, R. PAUL DRAKE, University of Michigan, CHAD MCCOY, TOM R. BOEHLY, University of Rochester, P-24 TEAM, DRAKE RESEARCH LAB TEAM, LABORATORY FOR LASER ENERGETICS TEAM — We present results of equation of state (EOS) measurement of carbon at a range of conditions falling into the warm dense matter (WDM) regime, solid density at temperatures ~ 1 – 10 eV. These conditions were created within diamond and graphite targets at the Omega laser facility. We employed a novel technique of laser driven shock and release, which produces different conditions from the Hugoniot states typically studied at high power laser facilities. These experiments take advantage of precise equation of state (EOS) measurements of shocked low density SiO2 aerogel foam used as pressure standard, which will also be presented. A simultaneous measurements of density, temperature and ionization state within the release wave were obtained from spatially resolved x-ray Thomson scattering, while the density and temperature measurements were bracketed by independent diagnostics including velocity interferometry, optical pyrometry and radiography, providing a full EOS measurement. Results will be compared with EOS models.

11:45AM J2.00004 Variational Perturbation Theory Path Integral Monte Carlo (VPT-PIMC): Trial Path Optimization Approach for Warm Dense Matter. JONATHAN BELOF, JONATHAN DUBOIS, Lawrence Livermore National Laboratory — Warm dense matter (WDM), the regime of degenerate and strongly coupled Coulomb systems, is of great interest due to it’s importance in understanding astrophysical processes and high energy density laboratory experiments. Path Integral Monte Carlo (PIMC) presents a particularly attractive formalism for tackling outstanding questions in WDM, in that electron correlation can be calculated exactly, with the nuclear and electronic degrees of freedom on equal footing. Here we present an efficient means of solving the Feynman path integral numerically by variational optimization of a trial density matrix, a method originally proposed for simple potentials by Feynman and Kleinert [Bachmann et al., Phys. Rev. A., 60:3429 (1999)], and we show that this formalism provides an accurate description of warm dense matter with a number of unique advantages over other PIMC approaches. An exchange interaction term is derived for the variationally optimized path, as well as a numerically efficient scheme for dealing with long-range electrostatics. Finally, we present results for the pair correlation functions and thermodynamic observables of the spin polarized electron gas, warm dense hydrogen and all-electron warm dense carbon within the presented VPT-PIMC formalism.

12:00PM J2.00005 Theoretical Predictions of Phase Transitions at Ultra-high Pressures. BRIAN BOATES, Dalhousie University, Lawrence Livermore National Laboratory — We present ab initio calculations of the high-pressure phase diagrams of important planetary materials such as CO2, MgSiO3, and MgO. For CO2, we predict a series of distinct liquid phases over a wide pressure (P) and temperature (T) range, including a first-order transition to a dense polymer liquid. We have computed finite-temperature free energies of liquid and solid CO2 phases to determine the melting curve beyond existing measurements and investigate possible phase separation transitions. The interaction of these phase boundaries with the mantle geotherm will also be discussed. Furthermore, we find evidence for a vast pressure-temperature regime where molten MgSiO3 decomposes into liquid SiO2 and solid MgO, with a volume change of approximately 1.2 percent. The demixing transition is driven by the crystallization of MgO – the reaction only occurs below the high-pressure MgO melting curve. The predicted transition pressure at 10,000 K is in close proximity to an anomaly reported in recent laser-driven shock experiments of MgSiO3. We also present new results for the high-pressure melting curve of MgO and its B1-B2 solid phase transition, with a triple point near 364 GPa and 12,000 K.

Tuesday, July 9, 2013 11:00AM - 12:15PM – Session J3 NT.1 Novel Techniques: Gun capabilities/Shock tubes
Fifth Avenue - William Buttler, Los Alamos National Laboratory

11:00AM J3.00001 Methods of Controlled Shock Wave Generation in A Shock Tube for Biological Applications. THUY-TIEN NGUYEN, JAMES WILGEROTH, WARREN MACDONALD, WILLIAM PROUD, Imperial College London, CENTRE FOR BLAST INJURY STUDIES, INSTITUTE OF SHOCK PHYSICS, IMPERIAL COLLEGE LONDON TEAM — The shock tube is a versatile and simple equipment used in a wide range of scientific research. The diaphragm breakage process, manipulated by different operation methods, is closely linked to the shock wave generated. Experiments were performed on a compressed air-driven shock tube with mylar and aluminium diaphragms of various thickness to characterise the output. The evolution of the pressure generated was measured and the diaphragm rupture investigated. Single-diaphragm and double-diaphragm configurations were employed, as were open or closed tube configurations. The arrangement was designed to enable high-speed photography and pressure measurements. Overall, results are highly reproducible, and show that the double-diaphragm system enables a more controllable diaphragm burst pressure. The diaphragm burst pressure was linearly related to its thickness within the range studied. The observed relationship between the diaphragm burst pressure and the generated shock pressure presents a noticeable difference compared to the theoretical ideal gas description. Furthermore, the duration of the primary shock decreased with the volume of the high-pressure charging gas. Computational modelling of the diaphragm breakage process was carried out using the ANSYS software package.
11:15AM J3.00002 Experiments on a Miniature Hypervelocity Shock Tube. DOUGLAS TASKER, CARL JOHNSON, MICHAEL MURPHY, MARK LIEBER, Los Alamos National Laboratory, MIMS TEAM — A miniature explosively-driven shock tube, based on the Voitkenko compressor design [1], has been designed to produce shock speeds in light gases in excess of 80 km/s. Voitkenko compressors over 1 meter in diameter have been reported but here experiments on miniature shock tubes with ~1-mm bore diameters are described. In this design a 12-mm diameter explosive pellet drives a metal plate into a hemispherical gas compression chamber. Downstream from the piston a mica diaphragm separates the gas from an evacuated shock tube which is confined by a massive polymethylmethacrylate (PMMA) block. The diaphragm eventually ruptures under the applied pressure loading and the compressed gases escape into the evacuated shock tube at hyper velocities. The progress of gas shocks in the tube and bow shocks in the PMMA are monitored with an ultra-high-speed imaging system, the Shock Wave Image Framing Technique (SWIFT) [2]. The resulting time-resolved images yield two-dimensional visualizations of shock geometry and progression. By measuring both the gas and bow shocks, accurate and unequivocal measurements of shock position history are obtained. The experimental results were compared with those of hydrocode modeling to optimize the design. The first experiments were suboptimum in that the velocities were ~16 km/s. Progress with these experiments will be reported.


11:30AM J3.00003 Non-Invasive Timing of Gas Gun Projectiles with Light Detection and Ranging1, PETER GOODWIN, Center for Integrated Nanotechnologies (MANTA), Los Alamos National Laboratory, MING WU, Sandia National Laboratory, DANA DATTELBAUM, Shock and Detonation Physics (WX-9), Los Alamos National Laboratory — We have developed a Light Detection and Ranging (LiDAR) diagnostic to track the position of a projectile inside of the gas gun barrel in real-time. This capability permits the generation of precisely timed trigger pulses useful for pre-triggering high-latency diagnostics such as a flash lamp-pumped laser. An initial feasibility test was performed using a 72 mm bore single-stage gas gun routinely used for dynamic research at Los Alamos National Laboratory. A 655-nm pulsed (~ 100 ps) diode laser operating at a pulse repetition rate of ~100 kHz was used to interrogate the position of the moving projectile in real-time. The position of the projectile in the gun barrel was tracked over a distance of ~3 meters prior to impact. The position record showed that the projectile moved at a constant velocity (483 m/s) prior to impacting the target. This velocity was in good agreement with independent measurements of the projectile velocity by photon Doppler velocimetry, and timing of the passage of the projectile through optical markers beams positioned at the muzzle of the gun. The LiDAR return can be processed in real-time to generate pre-trigger pulses at preset separations between the projectile and target.

1Work funded by LANL Laboratory Directed Research Project 2011012DR. LA-UR-13-21121, approved for public release.

11:45AM J3.00004 Sample Preheating Capability for Dynamic Material Studies*, J. L. WISE, D. C. DALTON, R. J. HICKMAN, Sandia National Laboratories, M. I. KAUFMAN, S. A. LEFFLER, M. J. JONES, National Security Technologies, LLC, J. J. LYNCH, A. C. BOWERS, Raytheon Ktech — Coordinated analysis, design, software development, hardware fabrication, and testing activities have yielded a new control system and experimental load design for dynamic material studies on specimens heated to temperatures exceeding 650°C prior to high-rate compression on a pulsed-power (e.g., Z machine) or gun platform. A proportional integral derivative controller supplies power for up to 16 resistive cartridge heaters mounted in a load assembly containing one or more test samples. The electrical output from this LabVIEW-based controller to each heater is continuously adjusted using feedback from thermocouples embedded in the load and in each heater. Experiments confirm steady temperature regulation to within ± 0.2°C of the selected set point, as well as adequate surge protection from built-in electromagnetic pulse isolation circuitry. ANSYS thermomechanical simulations have guided the refinement of load design to minimize sample temperature gradients and thermal distortion. Improved thin-film coatings for the sample/window interface are being developed to ensure the viability of velocity interferometry measurements on preheated samples. *Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

12:00PM J3.00005 Use of synchrotron radiation for research of flow of a products of detonation. LEV MERZHIEVSKY, E. R. PRUJEL, K. A. TEN, V. M. TITOV, L. A. LUK YANCHIKOV, E. B. SMIRNOV, A. K. MUZIRYA, Lavrentiev Institute of Hydrodynamics SB RAS — Results of studying detonation processes in condensed high explosives, which are obtained by methods based on using synchrotron radiation, are given. Data on the density distribution in the detonation front and behind the front for several high explosives are presented. Spatial distribution of density of products of a detonation, and values of parameters in the Neumann spike and at the Jouguet point are determined. A method of reconstruction of the distributions of gasdynamic characteristics of the flow of products of a detonation (density fields, particle velocity vector, and pressure) in the space was proposed and tested. Results of using this method for studying detonation of a charge of TNT and plasticbonded TATB are presented. The obtained data are a basis for determination of parameters of the equations of state of products of a detonation.

Tuesday, July 9, 2013 11:00AM - 12:30PM
Session J4 TM First Principles Methods IV Vashon - Richard Needs, University of Cambridge

11:00AM J4.00001 Equations of State for Mixtures: Results from DFT Simulations of Xenon/Ethane Mixtures Compared to High Accuracy Validation Experiments on Z, RUDOLPH MAGYAR, Computational Shock and Multiphysics Department, Sandia National Laboratories — We report a computational and validation study of equation of state (EOS) properties of liquid / dense plasma mixtures of xenon and ethane to explore and to illustrate the physics of the molecular scale mixing of light elements with heavy elements. Accurate EOS models are crucial to achieve high-fidelity hydrodynamics simulations of many high-energy-density phenomena such as inertial confinement fusion and strong shock waves. While the EOS is often tabulated for separate species, the equation of state for arbitrary mixtures is generally not available, requiring properties of the mixture to be approximated by combining physical properties of the pure systems. The main goal of this study is to access how accurate this approximation is under shock conditions. Density functional theory molecular dynamics (DFT-MD) at elevated-temperature and pressure is used to assess the thermodynamics of the xenon-ethane mixture. The simulations are unbiased as to elemental species and therefore provide comparable accuracy when describing total energies, pressures, and other physical properties of mixtures as they do for pure systems. In addition, we have performed shock compression experiments using the Sandia Z-accelerator on pure xenon, ethane, and various mixture ratios thereof. The Hugoniot results are compared to the results obtained from the DFT-MD simulations. These results show that DFT-MD simulations compare well with the experimental points, and it is found that a mixing rule based on pressure equilibration performs reliably well for the mixtures considered.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
and the validity of this test is explored with modeling and basic theory. Compared with formulations using LiF as an inert surrogate replacement for Al, the results are compared with other near-field blast tests and cylinder tests, particularly at different charge sizes and charge timescales using piezoelectric pencil gauges. Specifically, tests have been performed with C4 to probe the contributions of ideal explosives and charge size to the imparted shock to the steel plate in the 50-300 microseconds timeframe, and are compared with free-field over-pressure measurements at 1.52 meters and millisecond timescales. Unconfined, 6.4 mm diameter rate-sticks were also utilized to determine the effect of Al compared to LiF on detonation velocity.

By comparison of the Al oxidation with LiF, data indicate that Al oxidation occurs on an extremely fast timescale, beginning and completing between 1 and 25 microseconds. Unconfined, 6.4 mm diameter rate-sticks were also utilized to determine the effect of Al compared to LiF on detonation velocity.

The porous Hugoniots for these materials were then analytically obtained and are validated by comparison with available data. Our calculations for TATB confirm the presence of a kink in the Hugoniots, and the softening of the shock response is explained in terms of a change in molecular conformation and the loss of aromaticity.

11:45AM J4.00003 Predicting the crystalline and porous equations of state for secondary explosives, Ryan Wixom, David Damm, Sandia National Laboratories — Accurate simulations of energetic material response necessitate accurate unreacted equations of state at pressures much higher than even the C-J state. Unfortunately, for reactive materials, experimental data at high pressures may be unattainable, and extrapolation from low-pressure data results in unacceptable uncertainty. In addition to being low-pressure, the available data is typically limited to the porous state. The fully-dense, or crystalline, equation of state is required for building mesoscale simulations of the dynamic response of energetic materials. We have used quantum molecular dynamics to predict the Hugoniots and 300K isotherms of crystalline PETN, HNS, CL-20 and TATB up to pressures not attainable in experiments. The porous Hugoniots for these materials were then analytically obtained and are validated by comparison with available data. Our calculations for TATB confirm the presence of a kink in the Hugoniots, and the softening of the shock response is explained in terms of a change in molecular conformation and the loss of aromaticity.

12:00PM J4.00004 Density Functional Theory Characterization of Potential Poly-Nitrogen Precursors, Ivan Oleynik, Aaron Landerville, Brad Steele, University of South Florida — The success of recovery of pure poly-nitrogen materials, such as cubic-gauche, from diamond anvil cells has proven both difficult and elusive. As it has been proposed that impurities within a polymeric nitrogen material can cause a dramatic increase in stability upon return of the material to ambient conditions, attention has turned to nitrogen-rich compounds, such as azides, as potential precursors to impure, but recoverable forms of poly-nitrogen compounds. To aid experimentalists in the search of novel poly-nitrogen compounds, thermo-physical properties and Raman spectra of the candidate precursor ammonium-azide, along with a theoretically predicted polymorph, are calculated using Density Functional Theory with and empirical van der Waals correction. Additionally, we present preliminary results for another proposed nitrogen-rich precursor cyanuric-triazide.

12:15PM J4.00005 Chemistry of Al in Oxidizer Medium: From Shock Initiation to Post Detonation Kinetics, Santanu Chaudhuri, Martin Losada, Shahayar Fotovati, ISP/Applied Sciences Laboratory, Washington State University — Reactive materials, propellants, and thermitics are often constructed from Al/oxidizer composites. Al/oxidizer composites are also considered for self-sustaining reactions for deep space applications to reduce the need for carrying oxygen. In particular, Al/Teflon, Al/I$_2$/O$_2$ and Al/RDX composites will be discussed as representative Al in oxidizer systems. Results of post-detonation kinetics using transition state theory and master equation based RRKM theory will be compared including discussion on some unresolved theoretical issues in collision theories and basis set effects in predicting the temperature/pressure-dependent kinetics. For Al/Teflon system, the RRKM theory calculated fall-off curves show a significant pressure dependence of rate constant in wide range of 0-1 MPa pressures at elevated temperatures. For Al/I$_2$/O$_2$, systems, incorporation of spin-orbit coupling in DFT with various standard and augmented basis sets is important. A mechanism for generation of I$_2$ and O$_2$ during the reaction will be proposed. Finally, describing shock initiation reactions inside a condensed phase Al/RDX composites for a combustion reaction or detonation is currently a challenge for theoretical chemistry and chemical dynamics community. Especially, exact theoretical treatment for kinetics of reactants in confined hot spots under high-pressure/temperature conditions is lacking. A new collision theoretical approach and reactive embedding possibilities will be discussed as alternative to reactive force field based simulations of hot-spot growth.

Tuesday, July 9, 2013 11:00AM - 12:30PM —
Session J5 EM.2 Nonconventional Energetics: Blast Effects

11:00AM J5.00001 Recent energetic materials research and capabilities at the centers, John Reynolds, Lawrence Livermore National Laboratory —

11:30AM J5.00002 High-Temperature and Pressure Aluminum Reactions in Carbon Dioxide Rich Post-Detonation Environments, Bryce Tappan, Virginia Manner, Steven Pemberton, Mark Lieber, Carol Johnsson, Eric Sanders, LANL — Powdered aluminum is a common additive to energetic materials, but little is understood regarding its reaction rate at very high temperatures and pressures in specific oxidizing gases such as carbon dioxide. Aluminum reaction kinetics in carbon dioxide have been studied in various reaction conditions, but difficulties arise in the more specific study of Al oxidation at the high pressures and temperatures in detonation reactions. To study these reactions, small particle size Al or the inert surrogate, LiF, was added to the energetic material benzotriifuroxan (BTF). BTF is a hydrogen-free material that selectively forms NO during the major oxidizing species for post-detonated Al oxidation. High-fidelity PIVD measurements were utilized for early wall velocity expression measurements in 12.7 mm copper cylinders. The JWL equation of state was solved to determine temperature, pressure and energies at specific time periods. A genetic algorithm was used in conjunction with a numerical simulation hydrocode, ALE3D, which enables the elucidation of aluminum reaction extent. By comparison of the Al oxidation with LiF data indicate that Al oxidation occurs on an extremely fast time scale, beginning and completing between 1 and 25 microseconds. Unconfined, 6.4 mm diameter rate-sticks were also utilized to determine the effect of Al compared to LiF on detonation velocity.

11:45AM J5.00003 Measurements of Near-Field Blast Effects with Kinetic Plates, Virginia Manner, Los Alamos National Laboratory, Steven Pemberton, None, Geoffrey Brown, Los Alamos National Laboratory, Stephanie Neuscammann, Lawrence Livermore National Laboratory, Bryce Tappan, Larry Hill, Daniel Preston, Los Alamos National Laboratory, Lee Glascoe, Lawrence Livermore National Laboratory — Few tests have been designed to measure the near-field blast impulse of ideal and non-ideal explosives, mostly because of the inherent experimental difficulties due to thermal effects on gauges and non-transparent fireballs. In order to measure blast impulse in the near field, a new test has been developed by firing spherical charges at 15.2 cm from steel plates and probing acceleration using laser velocimetry. Tests measure the velocity imparted to the steel plate in the 50-300 microseconds timeframe, and are compared with free-field over-pressure measurements at 1.52 meters and millisecond timescales using piezoelectric pencil gauges. Specifically, tests have been performed with C4 to probe the contributions of ideal explosives and charge size effects. Non-ideal aluminumic explosive formulations have been studied to explore the role of aluminum in near-field blast effects and far-field pressure, and are compared with formulations using LiF as an inert surrogate replacement for Al. The results are compared with other near-field blast tests and cylinder tests, and the validity of this test is explored with modeling and basic theory.
12:00PM J5.00004 Numerical Simulations of Near-Field Blast Effects using Kinetic Plates, STEPHANIE NEUSCAMMAN, Lawrence Livermore National Laboratory, VIRGINIA MANNER, GEOFFREY BROWN, Los Alamos National Laboratory, LEE GLASCOE, Lawrence Livermore National Laboratory — Numerical simulations using two hydrocodes were compared to near-field measurements of blast impulse associated with ideal and non-ideal explosives to gain insight into testing results and predict untested configurations. The recently developed kinetic plate test was designed to measure blast impulse in the near-field by firing spherical charges in close range from steel plates and probing plate acceleration using laser velocimetry. Plate velocities for ideal, non-ideal and aluminized explosives tests were modeled using a three dimensional hydrocode. The effects of inert additives in the explosive formulation were modeled using a 1-D hydrocode with multiphase flow capability using Lagrangian particles. The relative effect of particle impact on the plate compared to the blast wave impulse is determined and modeling is compared to free field pressure results. This work is performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This is abstract LLNL-ABS-622152.

12:15PM J5.00005 Effect of Aluminium Confinement on ANFO Detonation, MARK SHORT, SCOTT JACKSON, CHARLES KIYANDA, MIKE SHINAS, STEVE HARE, MATT BRIGGS, Los Alamos National Lab — Detonations in confined non-ideal high explosives often have velocities below the confiner sound speed. The effect on detonation propagation of the resulting subsonic flow in the confiner (such as confiner stress waves traveling ahead of the main detonation front or upstream wall deflection into the HE) has yet to be fully understood. Previous work by Sharpe and Bdzil (J. Eng. Math, 2006) has shown that for subsonic confiner flow, there is no limiting thickness for which the detonation dynamics are uninfluenced by further increases in wall thickness. The critical parameters influencing detonation behavior are the wall thickness relative to the HE reaction zone size, and the difference in the detonation velocity and confiner sound speed. Additional possible outcomes of subsonic flow are that for increasing thickness, the confiner is increasingly deflected into the HE upstream of the detonation, and that for sufficiently thick confiners, the detonation speed could be driven up to the sound speed in the confiner. We report here on a further series of experiments in which a mixture of ammonium nitrate and fuel oil (ANFO) is detonated in aluminum confiners with varying HE charge diameter and confiner thickness, and compare the results with the outcomes suggested by Sharpe and Bdzil.

Tuesday, July 9, 2013 11:00AM - 12:15PM —
Session J6 EM.1 Ignition II Cascade II - Harold Sandusky, Naval Surface Warfare Center - Indian Head

11:00AM J6.00001 Initiation Mechanisms in IHE and CHE Materials, ANDREW JARDINE, DAVID WILLIAMSON, STEPHEN WALLEY, University of Cambridge, STEWART PALMER, Retired, CLAIRE LEPPARD, AWE, Aldermaston, FRACTURE & SHOCK PHYSICS GROUP, UNIVERSITY OF CAMBRIDGE TEAM, AWE TEAM — Impact sensitivity and subsequent impact initiation is one of the key characteristics of explosive materials. Various standardised tests exist, such as the Rotter or BAM impact tests, which allow the relative sensitivity of different materials to be characterised. However, these provide little insight into the underlying behaviour of the material. The use of a periscopic glass-anvil drop-weight apparatus has proven to provide valuable information about the hotspot initiation of many materials [1,2]. In this paper we describe experiments which apply the technique, in conjunction with high speed video and additional diagnostic instrumentation, to study the mechanism of initiation of modern explosive materials including TATB, LLM-105, Fox-7, HMX, RDX and PETN.


11:15AM J6.00002 A framework for analyzing the ignition response of energetic materials under dynamic loading, SEOKPUM KIM, ANANDA BARUA, MIN ZHOU, Georgia Institute of Technology — A multiphysics finite element framework is developed to analyze the ignition response of energetic materials under dynamic loading. The framework uses a cohesive finite element method (CFEM) to capture large deformation, microcracks, and frictional heating. Chemical reactions are incorporated into this framework by accounting for the decomposition of energetic granules according to chemical kinetic models. As an application, the dynamic response of HMX-Estane polymer-bonded explosive (PBX) is analyzed. The focus is on the effect of loading intensity and microstructural attributes on hot spot evolution, coalescence, and ignition. Results suggest that the time taken to form critical hotspots (order of microseconds) from thermo-mechanical dissipation processes is several orders of magnitude smaller than the time taken for ignition to occur (order of milliseconds). Microstructure-performance relations obtained from this analysis can be used to design explosives with tailored attributes and safety envelopes.

11:30AM J6.00003 Modeling pore collapse and chemical reactions in shock-loaded HMX crystals, RYAN AUSTIN, NATHAN BARTON, WILLIAM HOWARD, LAURENCE FRIED, Lawrence Livermore National Laboratory — The collapse of micron-sized pores in crystalline high explosives is the primary route to initiating thermal decomposition reactions under shock wave loading. Given the difficulty of resolving such processes in experiments, it is useful to study pore collapse using numerical simulation. A significant challenge that is encountered in such calculations is accounting for anisotropic mechanical responses and the effects of highly exothermic chemical reactions. In this work, we focus on simulating the shock-wave-induced collapse of a single pore in crystalline HMX using a multiphysics finite element code (ALE3D). The constitutive model set includes a crystal-mechanics-based model of thermoelastic-viscoplasticity and a single-step decomposition reaction with empirically determined kinetics. The model is exercised for shock stresses up to ~10 GPa to study the localization of energy about the collapsing pore and the early stages of reaction initiation.

2This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-618941).
11:45AM J6.00004 Large-Scale Atomic Simulation of Shock-induced Initiation Processes in Energetic Materials1. AIDAN THOMPSON, Sandia National Laboratories — Initiation in energetic materials is fundamentally dependent on the interaction between a host of complex chemical and mechanical processes, occurring on scales ranging from intramolecular vibrations through molecular crystal plasticity up to hydrodynamic phenomena at the mesoscale. A variety of methods (e.g., quantum electronic structure methods (QM), non-reactive classical molecular dynamics (MD), mesoscopic continuum mechanics) exist to study processes occurring on each of these scales in isolation, but cannot describe how these processes interact with each other. In contrast, the ReaxFF reactive force field, implemented in the LAMMPS parallel MD code, allows us to routinely perform multimillion-atom reactive MD simulations of shock-induced initiation in a variety of energetic materials. This is done either by explicitly driving a shock-wave through the structure (NEMD) or by imposing thermodynamic constraints on the collective dynamics of the simulation cell e.g. using the Multiscale Shock Technique (MSST). These MD simulations allow us to directly observe how energy is transferred from the shockwave into other processes, including intramolecular vibrational modes, plastic deformation of the crystal, and hydrodynamic jetting at interfaces. These processes in turn cause thermal excitation of chemical bonds leading to initial chemical reactions, and ultimately to exothermic formation of product species. Results will be presented on the application of this approach to several important energetic materials, including pentaerythritol tetranitrate (PETN) and ammonium nitrate/fuel oil (ANFO).

In both cases, we validate the ReaxFF parameterizations against QM and experimental data. For PETN, we observe initiation occurring via different chemical pathways, depending on the shock direction. For PETN containing spherical voids, we observe enhanced sensitivity due to jetting, void collapse, and hotspot formation, with sensitivity increasing with void size. For ANFO, we examine the effect of reaction rates on shock direction, fuel oil fraction, and crystal/fuel oil/void microstructural arrangement.

Tuesday, July 9, 2013 11:00AM - 12:30PM – Session J7 CM.2 Phase Transitions: Structural Transitions I Grand Crescent - C.S. Yoo, Washington State University

11:00AM J7.00001 Pressure-induced phase transformation of In$_3$Se$_3$. ANYA RASMUSSEN, SAMUEL TEK-LEMICHAEL, ELHAM MAFI, YI GU, MATTHEW MCCLUSKEY, Washington State University — Phase-change memory, with fast read-write speeds and small dimensions, will soon replace flash memory in our cell phones and tablets. This type of memory relies on phase change materials like indium selenide, In$_3$Se$_3$, a III-VI semiconductor that exists in multiple crystalline phases. To achieve controlled switching between phases, it is important to understand both the thermal and elastic properties of In$_3$Se$_3$. Using synchrotron x-ray diffraction and a diamond-anvil cell, a pressure-induced phase transition in powder In$_3$Se$_3$ from the α phase to β phase was discovered at 0.7 GPa. This pressure is an order of magnitude lower than phase-transition pressures in most semiconductors. Raman spectroscopy experiments confirm this result. The bulk moduli are reported for both α and β phases, and the c/a ratio for the β phase is shown to have a nonlinear dependence on pressure.

11:15AM J7.00002 High pressure study of group-IV clathrate by XRD and Raman scattering. TETSUJI KUME, SHIGEO SASAKI, Gifu University — Group-IV clathrates, which are open-structured Si, Ge, and Sn cage-like compounds, have attracted increasing attention because of their potential applications for thermoelectric devices due to the behavior of phonon-glass and electron-crystal. One of the keys for the intriguing properties is so called rattling vibrations of guests. The direct observation of the rattling is important for understanding of the clathrate properties. Furthermore, the systematic observations of the rattling vibrations as a function of the cage size controlled by pressure are very significant to investigate the guest-host interaction. The pressurization also throws light on the structural stability of the clathrate, which is improved by the guest atoms. The clathrate structure with sp$^3$ network is preserved up to very high pressure. Instead of the structural change, the doped Si clathrates undergo an isostructural phase transition. This paper is concerned with the structural stabilities under high pressure and the rattling vibrations of the guest as a function of the cage size, investigated for various semiconductor clathrates (Si$_4$Ga$_2$Ge$_5$Sb$_2$Ge$_3$, Eu$_4$Ga$_2$Ge$_5$Sb$_2$Ge$_3$, and so on) by means of Raman and XRD experiments. On the recent data, the guest-host interaction is discussed.

11:30AM J7.00003 Pressure effect on the isostructural transition in RNiAl compounds (R=Tb and Gd). JIRI PRchal, MILAN KLIČPERA, PETR DOLEZAL, JIRI KASTIL, MARTIN MISEK, PAVEL JAVORSKY, Charles University in Prague, DCMP — TbNiAl and GdNiAl belong to a large group of compounds crystallizing in the hexagonal ZnNiAl-type of structure. Within recent years, physics of the discontinuity in the temperature or composition dependence of the lattice parameters [a and c] observed in several compounds of this family of intermetallics has been of particular interest. These materials have in common a specific ”forbidden” value of the c/a ratio. This conclusion has been corroborated by ab initio calculations [1]. Although the dramatic structure change is hardly observable in the temperature dependence of the specific heat, it is accompanied with a clear change of the effective magnetic moment, change of the crystal field energy spectra [2] and namely with increasing amount of mechanical defects in the sample. TbNiAl as a representative of such behavior, exhibits a first-order structural transition at low temperatures around 100K [3]. We have for the first time studied this structural step upon application of hydrostatic pressure on both – poly- and monocystal of TbNiAl and a polycrystalline GdNiAl, in which the structural step appears still higher around 240K. Our experimental observation of an unusually rapid decrease of the critical temperature with pressure will be discussed in terms of differences of the intra- and interplanar chemical bonding in this type of structure. [1] J. Prchal et al., Phys. Rev. B 77 (2008) 134106. [2] P. Javorsky et al., J Magn. Magn. Mat. 317 (2007) e400. [3] J. Prchal et al., Physica B 378-380 (2006) 1102.

11:45AM J7.00004 Pressure Induced Phase Transitions of Yb: NaBi(WO$_4$)$_2$ up to 51 GPa. HANG CUI, CHUNLI MA, XIAOXIN WU, HONGYANG ZHU, HONGDONG LI, QILANG CUI, Jilin University, PR China — High-pressure Raman scattering and luminescence spectra studies have been performed on Yb: NaBi(WO$_4$)$_2$ up to 51 GPa at room temperature by using diamond anvil cell techniques. The Yb-doped single crystals of scheelite double tungstates NaBi(WO$_4$)$_2$ have been grown by Czochralski method. High-pressure Raman scattering results indicate that Yb: NaBi(WO$_4$)$_2$ undergoes phase transition from tetragonal (I4 1/a) to monoclinic (I2/a) symmetry at around 6.5 GPa. When the pressure reaches to 23.3 GPa, the color of sample changes from yellow to red observed by optical microscope, and the luminescence spectra is dramatically different from the thermal phase, it is indicated that the energy level transition maybe occurs around this pressure. With pressure is higher than 32.1 GPa, the color of sample changes from yellow to red observed by optical microscope, and the luminescence spectra is dramatically different from the previous one. The luminescence spectra of Yb: NaBi(WO$_4$)$_2$ is mainly consists of 4f-4f transitions, which is very sensitive to the crystal field energy of 4f states, we can conclude that the Yb: NaBi(WO$_4$)$_2$ may be used as a pressure sensor.

1This work was supported by the NSF of China (91019004, 11004074, 11074089), the specialized Research Fund for the Doctoral Program of Higher Education (2010061110011, 2010061120059), and the National Basic Research Program of China (2011CB808200).
12:00PM J7.00005 On the phase diagrams of the helimagnets MnSi and Cu$_2$OSeO$_3$ — SERGEI M. STISHOV, ALLA E. PETROVA, V.A. SIDOROV, Institute for High Pressure Physics of Russian Academy of Sciences — A series of resistivity measurements on a MnSi single crystal was performed at high pressures, created by a piston-cylinder device with a liquid pressure medium. The form of the resistivity curve at ambient pressure clearly indicates a first order nature of the magnetic phase transition in MnSi. Application of high pressure rapidly degrades the first order features of the phase transition. The temperature derivative of resistivity demonstrates two notable features of the phase transition that disappear on increasing pressure: a sharp peak marking the first order phase transition and a shallow maximum situated slightly above the critical temperature and pointing to prominent helical fluctuations. The current experimental data rule out any strong first order phase transition in MnSi at high pressures and low temperatures, which would prevent development of a quantum critical region. On the contrary, there should exist true quantum critical phenomena in MnSi at high pressures because a weak first order transition, if it survives at high pressures to the lowest temperatures, should not suppress the entire quantum critical region. Recently a dielectric compound Cu$_2$OSeO$_3$ possessing a cubic non-centro symmetric P2$_1$3 crystal structure, like MnSi, was found to have a magnetic structure and T-H magnetic diagram similar to those of MnSi [1]. We have studied the magnetic transition in this material by means of magnetic ac-susceptibility and ac-calorimetry at nearly hydrostatic pressure up to 6 GPa. The data obtained are analyzed in hope to understand the nature of the chiral fluctuation region adjacent to the helical phase transitions.

12:15PM J7.00006 Second harmonic generation measurements for the determination of pressure induced phase transitions — LKHAMSUREN BAYARJARGAL, BJÖRN WINKLER, Goethe University — We show that optical second harmonic generation measurements can be used to efficiently delineate phase boundaries in high pressure experiments in diamond anvils and understand transition pathways. We have employed SHG measurements to study the pressure-induced structural phase transitions in AlN and ZnO as a function of temperature and of particle size. Furthermore, we demonstrate that pressure-induced magnetic phase transitions can be detected by this approach and show that the transition from an antiferromagnetic to a centrosymmetric magnetic structure occurs in Cu$_2$OSeO$_3$ at 10(1) GPa. The pressure dependence of the Neel temperature, $dT_N/dp = -1.0(2)$ K/GPa from our SHG measurements, which differs significantly from earlier results where $dT_N/dp$ ranged from -16 K/GPa to +15 K/GPa. Further examples, where SHG measurements have provided information on pressure induced structural phase transitions are the cases of KIO$_3$, where two transitions at 7 and 14 GPa were identified, and of ice VII, where SHG measurements do not support a proposed acentric high pressure modification.

Tuesday, July 9, 2013 1:45PM - 3:00PM — Session K1 ME.3 Inelastic Deformation, Fracture, and Spall II Grand Ballroom I - K.T. Ramesh, Johns Hopkins University

1:45PM K1.00001 Influence of shock loading kinetics on the spall response of copper — JUAN ESCOBEDO, DARCEY DENNIS-KOLLER, ELLEN CERETTA, BRIAN PATTSON, CURT BRONKHORST, Los Alamos National Laboratory — A suite of plate-impact experiments was designed and conducted to examine the influence of loading kinetics on the spall response of high purity copper samples. The density of grain boundaries dynamically loaded and peak compressive stresses (1.5GPa) were held constant for all experiments. The kinetics of the tensile pulses were designed using a hydrodynamic shock-wave propagation code and experimentally achieved by controlling the geometry of copper impactors and targets. Examination of damage fields shows that the total fraction of damage (voids) decreases as the tensile rates increase. In addition, an accompanying larger plastic dissipation, in the form of grain misorientation measured by means of electron backscatter diffraction, is present in the samples deformed at lower tensile rates. These results suggest a time dependent behavior of the processes that convert plastic dissipation into void growth.

2:00PM K1.00002 High temperature impact response of copper — EUGENE ZARETSKY, Ben-Gurion University, Israel, GENNADY KANEL, Institute for High Temperatures, Russia — The evolution of elastic-plastic shock waves with the propagation distance has been studied in 99.999-% purity polycrystalline copper. The free surface velocity histories of 0.1 to 2.0 mm thick samples shock-loaded from initial temperatures 300 to 1353 K, have been recorded using VISAR. Experiments confirmed anomalous growth of the HEL value with temperature. With approaching melting temperature the growth becomes stronger while the shape of the elastic precursor wave changes and becomes spike-like. These changes are possibly caused by the increase of the amount of lattice defects near melting. Results of measurements of the precursor decay at different initial temperatures have been converted into relationships between the shear stress and the initial plastic strain rate at the top of the precursor wave. The strain rate was found to decrease over 0.25 to 2-mm precursor traverse from $2 \times 10^4$ to $6 \times 10^3$ s$^{-1}$ at 1353 K and from $7 \times 10^3$ to $2.3 \times 10^3$ s$^{-1}$ at 300 K. An analysis of the rise times of the plastic shock waves has shown that for the same level of shear stress, the plastic strain rate at the shock front at 300 K is by a factor of 300 and at 1353 K is by a factor of 30 higher than just behind the elastic precursor front.

2:15PM K1.00003 A Comparison of Multiple Techniques for Determining the Release Behaviour of a Simple FCC Metal — MICHAEL LOWE, AWE, Aldermaston, DAVID CHAPMAN, Institute of Shock Physics, Imperial College London, STEVE ROTHMAN, CHRIS ROBINSON, AWE, Aldermaston — A shock compression pulse normally consists of a discontinuous rise in stress or pressure followed by a sustained period, if loaded using a technique such as plate impact, and terminated with a release back to ambient conditions over a finite time. Although historically a great body of work has been undertaken on the measurement and characterisation of the rise profile and plateau of many metals, minerals and other materials, the subsequent release phenomenon has tended not to be so vigorously investigated. This release behaviour is a compound effect, normally dependent upon the initial shock loading conditions and the distance within the subject material that the subsequent release effect has travelled. We discuss recent work undertaken on the development and testing of methodologies for investigating the release behaviour. These methods were employed to determine the release behaviour of a commonly available commercial C101 copper, the choice of which was made to minimise experimental complications due to any phase changes, microstructural effects or inherent material strength.

2:30PM K1.00004 On the homogenous nucleation and propagation of dislocations under shock compression — HUSSEIN ZBIB, Washington State University — In strong shock regimes, homogenous nucleation of dislocation loops is believed to be the dominant mechanism of plastic deformation. We compare threshold stress for homogenous nucleation calculated by continuum elasticity and standards nucleation theory with multiscale dislocation dynamics plasticity (MDDP) predictions for copper single crystals. Several MDDP homogenous nucleation simulations are then carried out to investigate the state of stress and strain behind the wave front. The results show that the stress filed exhibits an elastic overshoot followed by rapid relaxation such that the1D state of strain is transformed into a 3D state of strain due to plastic flow. Based on MDDP results, we develop models for dislocation density evolution, saturated dislocation density, and stress relaxation time at different pressures. Moreover, an extension of high strain rate Orowan equation that accounts for homogenous nucleation is derived. The dependence of strain rate on the peak pressure shows good agreement with Swegle-Grady scaling law.

1 and Mutasem A. Shehadeh, American University of Beirut

Tuesday, July 9, 2013 1:45PM - 3:15PM — Session K2 CM.1 Equation of State: Experimental Methods Grand Ballroom II - Paulo Rigg, Los Alamos National Laboratory
Optical methods for determining the shock Hugoniot of Solids

Expansion of temperature measurement at lead/LiF interface under shock compression

An examination of material strength, phase boundaries and hysteresis through continuous measurements of release isentropes

Velocity correction and refractive index changes for [100] lithium fluoride optical windows under isentropic compression

A new method to study he effective shear modulus of shocked material

Versatile target assembly of explosive loading experiments for measuring sound velocity under high pressure: copper and bismuth as examples

Tuesday, July 9, 2013 1:45PM - 3:00PM
Session K3 TM First Principles Methods V Fifth Avenue - Rudy Magyar, Sandia National Laboratories
1:45PM K4.00001 Nitrogen-rich mixtures for high-energy density applications, AMANUEL TEWELDEBERHAN, Lawrence Livermore National Lab — Nitrogen transforms from molecular to polymeric phase at high pressure. Polymeric nitrogen is one of the most studied candidates for high energy density materials. There is an interesting question of whether introducing small amounts of impurities can alter the polymerization to lower pressures and lead to enhanced metastability. To address this, we have used first-principles density functional theory to study the electronic, structural, and dynamical properties of nitrogen-rich mixtures. We have identified several solid phases for different nitrogen concentrations and investigated the thermodynamic stability of solid and liquid mixtures with respect to their pure components.

1Work supported by LLNL. Prepared by LLNL under Contract DE-AC52-07NA27344.

2:15PM K4.00002 Achieving accuracy in first-principles calculations at extreme temperature and pressure, ANNE E. MATTSSON, Sandia National Labs, JOHN M. WILLS, Los Alamos National Laboratory — First-principles calculations are increasingly used to provide EOS data at pressures and temperatures where experimental data is difficult or impossible to obtain. The lack of experimental data, however, also precludes validation of the calculations in those regimes. Factors influencing the accuracy of first-principles data include theoretical approximations, and computational approximations used in implementing and solving the underlying equations. The first category includes approximate exchange-correlation functionals and wave equations simplifying the Dirac equation. In the second category are, e.g., basis completeness and pseudo-potentials. While the first category is extremely hard to assess without experimental data, inaccuracies of the second type should be well controlled. We are using two rather different electronic structure methods (VASP and RSPt) to make explicit the requirements for accuracy of the second type. We will discuss the VASP Projector Augmented Wave potentials, with examples for Li and Mo. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:30PM K4.00003 Achieving accuracy in first-principles calculations for EOS: basis completeness at high temperatures, JOHN M. WILLS, Los Alamos National Laboratory, ANNE E. MATTSSON, Sandia National Laboratories — First-principles electronic structure calculations can provide EOS data in regimes of pressure and temperature where accurate experimental data is difficult or impossible to obtain. This lack, however, also precludes validation of calculations in those regimes. Factors that influence the accuracy of first-principles data include (1) theoretical approximations and (2) computational approximations used in implementing and solving the underlying equations. In the first category are the approximate exchange/correlation functionals and approximate wave equations approximating the Dirac equation; in the second are basis completeness, series convergence, and truncation errors. We are using two rather different electronic structure methods (VASP and RSPt) to make definitive the requirements for accuracy of the second type, common to both. In this talk, we discuss requirements for converged calculation at high temperature and moderated pressure. At convergence we show that both methods give identical results. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:45PM K4.00004 Z methodology for phase diagram studies: tantalum and platinum as examples, LEONID BURAKOVSKY, DEAN PRESTON, SHAO PING CHEN, DANIEL SHEPPARD, Los Alamos National Laboratory, Z-TEAM — Z methodology is a novel technique for phase diagram studies. It combines direct Z method for the calculation of melting curves, and inverse Z method for the calculation of solid-solid phase boundaries. Relative solid phase stability is studied by comparing melting curves of different solid phases to determine which one is the highest, and thus which of the corresponding solid phases is the most stable. In the inverse Z method, the equilibrium phase is determined by freezing liquid into the most stable solid phases on both sides of the phase boundary. Inverse Z method represents the implementation of this approach in terms of ab initio molecular dynamics using VASP package. We will discuss the application of Z methodology to the study of the phase diagrams of tantalum and platinum, and compare our results to the most recent experimental data.

Tuesday, July 9, 2013 1:45PM - 3:15PM — Session K4 NM.1 Superhard Materials — Vashon - Toshimori Sekine, Hiroshima University

1:45PM K4.00001 Elastic moduli of hard c-Zr$_3$N$_4$ and γ-Ta$_2$N$_3$, a tough self-healing material, via laser ultrasonics and nanoindentation, ANDREAS ZERR, LPSP-CNRS, Villeteaune, France, NIKOLAY CHIGAREV, LAUM, Universite du Maine, Le Mans, France, JUDITH BOURGUILLE, FLORENT TETARD, OVIDIU BRINZA, SERGEY NIKITIN, LPSP-CNRS, Villetaune, France, ALEXEY LOMONOSOV, Institute of General Physics, Moscow, Russia, VITALIY GUSEV, IMM, Universite du Maine, Le Mans, France — Bulk and shear moduli ($B_0$ and $G_0$) of the dense polycrystalline oxygen-bearing c-Zr$_3$N$_4$ and γ-Ta$_2$N$_3$ were determined from the laser ultrasonic (LU) measurements on highly porous samples having the volume fraction porosity of 0.23 and 0.18, respectively. Dense samples of these high-pressure (HP) materials are today not available due to their very high hardness and absence of a densification procedure. Combining the LU data with a numerical analysis of the sample porosity, the “true” isotropic moduli were determined to be $B_0 = 217(20)$ GPa and $G_0 = 163(9)$ GPa, for c-Zr$_3$N$_4$, and $B_0 = 240(15)$ GPa and $G_0 = 123(2)$ GPa, for γ-Ta$_2$N$_3$. For both HP-nitrides the $B_0$ values agree with those obtained earlier via the HP compression measurements in a diamond anvil cell. Also, the self-healing behavior of γ-Ta$_2$N$_3$ by mechanical polishing was confirmed by two independent methods. Finally, the results obtained for γ-Ta$_2$N$_3$ via the LU method were compared with our nanoindentation measurements. The high $G_0$ value of c-Zr$_3$N$_4$ suggests that this material could vie with γ-Si$_3$N$_4$ for the rank of the third hardest material after diamond and c-BN.

1Supported by the Agence Nationale de la Recherche (France).

2:00PM K4.00002 Industrial scale HP-HT synthesis of hard and wear resistant c-Zr$_3$N$_4$, DMYTRO DIZVENKO, RALF RIEDEL, TU Darmstadt, Germany, TAKASHI TANIGUCHI, NIMS, Tsukuba, Japan, THIERRY CHAUVEAU, ANDREAS ZERR, LPSP-CNRS, Villetaune, France — We present a large scale high-pressure high-temperature (HP-HT) synthesis of hard and wear resistant cubic zirconium nitride having Th$_3$P$_4$-type structure, c-Zr$_3$N$_4$. This material, also available as well-adhesive coatings with exceptional wear resistance, represents a compound competitive to diamond and c-BN with respect to machining of low-carbon steels and other ferrous alloys. We obtained c-Zr$_3$N$_4$ powder at pressures as low as 6.5 GPa and temperatures of 1400-1600 °C from nanocrystalline Zr$_3$N$_4$ powder using a belt-type apparatus – a static HP-HT device widely employed for the commercial production of diamond and c-BN. The HP products are characterized in detail by means of powder X-ray diffraction, Raman spectroscopy, scanning electron microscopy and combustion elemental analysis. In addition to major polycrystalline c-Zr$_3$N$_4$, we unveil the formation of a quaternary compound c-(Zr$_1-x$Ta$_x$)$_3$N$_4$ which indicates the possibility of doping of c-Zr$_3$N$_4$, thus introducing it for practical application as a multifunctional material. Moreover, we consider ways of cementing the c-Zr$_3$N$_4$ powders (similar to cemented tungsten carbides) which would allow economic fabrication of large bodies based on this compound.

2Supported by the DFG (Bonn, Germany) within SPP 1236 and by the IFR “Paris Nord Plaine de France.”
2:15PM K4.00003 Shock Syntheses of Novel Nitrides and Biomolecules, ToshiMori Sekine, Hiroshima University — High-pressure spinel nitride of Si3N4 was discovered more than 10 years ago. Since then there have been many studies on the spinel nitrides and related materials including oxynitrides. We have developed shock synthesis method to investigate their structural, mechanical, chemical, physical, and optical properties. At the same time we tried to synthesize carbon nitrides from the organic substances. And later we extended to shock synthesis of ammonia through the Haber-Bosch reaction under shock in order to apply geochemical subjects related to the origin of life. The simplest amino acid of glycine, as well as amines (up to propylamine) and carboxylic acids (up to pentanoic acid), has been synthesized successfully in aqueous solutions through meteorite impact reactions. Recently we are trying to make more complex biomolecules for implications of biomolecule formation for the origin of life through meteorite impacts on early Earth’s ocean. These results of shock syntheses may imply significant contributions to materials science and Earth and planetary sciences. This research is collaborated with National Institute for Materials Science and Tohoku University.

2:45PM K4.00004 Structural change in hBN coexisting with hydrogen gas under pressure, Atsuko Nakayama, Center for Transdisciplinary Research, Niigata University, Shotaro Taguchi, Graduate School of Science & Technology, Niigata University, Shohei Mitsuya, Department of Physics, Faculty of Science, Niigata University, Takashi Taniguchi, Satoshi Nakano, National Institute for Materials Science (NIMS), Ayako Ohmura, Center for Transdisciplinary Research, Niigata University, Fumihiro Ishikawa, Yuh Yamada, Department of Physics, Faculty of Science, Niigata University — Hexagonal boron nitride (hBN) has the layered structure as graphite, while the magnitude of band gaps is very large (~0.5 eV). It is thought that hBN hardly causes charge transfer interaction with any atoms or molecules. On the other hand we examined pressure-induced structural-changes in multi-walled carbon-nanotubes (MWCNTs) and meso-carbon micro-beads (MCMs) coexisting with hydrogen gas using a diamond anvil cell (DAC) at room temperature. Both of them showed abnormal pressure dependence of in-plane graphite-structure, suggesting intercalation of hydrogen. Then we thought hBN has also possibility to cause the intercalation of hydrogen using pressure. In this study x-ray diffraction of hBN coexisting with hydrogen was carried out at room temperature to investigate the pressure-induced intercalation of hydrogen from the point of view of structural study. Not only the interlayer distance but also the a-axis length show abnormal pressure dependence up to ~1.5 GPa. In particular the a-axis length increases with increasing the pressure in the range between 1 and 1.5 GPa. According to the relatively-low quantitative-reproducibility of change, it is thought that the hBN-hydrogen system takes an un-steady and non-equilibrium state.

3:00PM K4.00005 Table-top Generation and Spectroscopic Study of ~10 TPa High-Energy Density Materials with C60 Hypervelocity (v ~ 100 km/s) Impact, Young Bae, Y.K. Bae Corporation — Intense bursts of soft x-rays were discovered by Bae et al. in hypervelocity (~100 km/s) impact of bio and water nanoparticles at the Brookhaven National Lab (BNL) in 1994. In the experiment, the nanoparticles were directly impacted on and detected by Si particle detectors that also detected the soft x-rays. Energy deposition measurements through thin films revealed that the impact generated pressures were ~10 TPa, and the photon energies in the range of 75-100 eV for Si targets. The conversion efficiency from the kinetic energy to the radiation energy was unexpectedly high, ~38%, which was attributed to Dicke Superradiance of collective quantum states in High-Energy Density Materials (HEDM), Metastable Innershell Molecular States (MIMS). This talk presents recent experimental results obtained in a table-top apparatus completely different from and orders of magnitude smaller than that at BNL. In the new setup, hypervelocity (~100 km/s) C60+ ions impacted on Al targets, and the impact generated soft x-rays were detected off-axis and analyzed using three Si photodiode detectors with selective energy response curves. The photon energy was determined to be ~70 eV with the kinetic-energy to photon-energy conversion efficiency of ~35% in confirmation of the results by Bae et al. at BNL. The present results demonstrate a new way of generation and spectroscopic study of HEDM with pressures exceeding 10 TPa, and show the pathway to scaling up the soft x-ray generation method for a wide range of applications from lithography to inertial fusion.

1 This work was supported by DTRA under the contract HDTRA1-12-C-0094.

Tuesday, July 9, 2013 1:45PM - 3:15PM — Session K5 EM.2 Nonconventional Energetic Materials

1:45PM K5.00001 Shock Initiation and Equation of State of Ammonium Nitrate, David Robbins, Steve Sheffield, Dana Dettelbaum, Raja Chellappa, Nenad Velisavljevic, Los Alamos National Laboratory — Ammonium nitrate (AN) is a widely used fertilizer and mining explosive commonly found in ammonium nitrate-fuel oil. Near AN is a non-ideal explosive with measured detonation velocities approaching 4 km/s. Previously, we reported a thermodynamically-complete equation of state for AN based on its maximum density, and showed that near-full density AN did not initiate when subjected to shock input conditions up to 22 GPa. In this work, we extend these initial results, by presenting new Hugoniot data for intermediate density neat AN obtained from gas gun-driven plate impact experiments. AN at densities from 1.8 to 1.5 g/cm3 were impacted into LiF targets and the unreacted EOS for AN was refined. Furthermore, shock initiation of neat AN was observed as the initial particle velocity profiles obtained for the lower density AN samples. At the same time we tried to synthesize carbon nitrides from the organic substances. And later we extended to shock synthesis of ammonia through the Haber-Bosch reaction under shock in order to apply geochemical subjects related to the origin of life. The simplest amino acid of glycine, as well as amines (up to propylamine) and carboxylic acids (up to pentanoic acid), has been synthesized successfully in aqueous solutions through meteorite impact reactions. Recently we are trying to make more complex biomolecules for implications of biomolecule formation for the origin of life through meteorite impacts on early Earth’s ocean. These results of shock syntheses may imply significant contributions to materials science and Earth and planetary sciences. This research is collaborated with National Institute for Materials Science and Tohoku University.

2:00PM K5.00002 Phase Diagram of Ammonium Nitrate, Mihindra Dunuwille, Choong-Shik Yoo, Department of Chemistry Washington State University and Institute for Shock Physics — Ammonium Nitrate (AN) has often been subjected to uses in improvised explosive devices, due to its wide availability as a fertilizer and its capability of becoming explosive with slight additions of organic and inorganic compounds. Yet, the origin of enhanced energetic properties of impure AN (or AN mixtures) is neither chemically unique nor well understood - resulting in rather catastrophic disasters in the past and thereby a significant burden on safety, in using ammonium nitrates even today. To remedy this situation, we have carried out an extensive study to investigate the phase stability of AN, in different chemical environments, at high pressure and temperature, using diamond anvil cells and micro-Raman spectroscopy. The present results confirm the recently proposed phase IV-to-IV’ transition above 15 GPa and provide new constraints for the melting and phase diagram of AN to 40 GPa and 673 K. Stephens, H.W. The Texas City disaster, 1947. Austin, TX: University of Texas Press. 1997 2: Alistair, J. D. et al., J. Phys. Chem. A 2011, 115, 11889; Dunuwille, M. et al., J. Phys. Chem. A 2012, 116, 7600.

1 The present study has been supported by the U.S. DHS under Award Number 2008-ST-061-ED0001.
2:15PM K5.00003 Detonation behavior of emulsion explosives sensitized with polymeric microbubbles. RICARDO MENDES, JOSÉ RIBEIRO, ADAI - Assoc. Devel, Aerodynamics Industrial; LEDAP- Lab. Energetics Detonics; Depart. of Mechanical Engineering, University of Coimbra, IGOR PLAKSIN, ADAI - Assoc. Devel. Aerodynamics Industrial; LEDAP- Lab. Energetics Detonics; Depart. of Mechanical Engineering; University of Coimbra, JOSÉ CAMPOS, ADAI - Assoc. Devel. Aerodynamics Industrial; LEDAP- Lab. Energetics Detonics; Depart. of Mechanical Engineering; University of Coimbra — The differences between the detonation behavior of ammonium nitrate based emulsion explosive sensitized with polymeric or with glass microbubbles is presented and discussed. Expancell® are hollow polymeric microbubbles that contain a hydrocarbon gas. The mean particle size of those particles is 30 µm and their wall thickness is about 0.1 µm. The detonation velocity and the failure diameter of the emulsion explosive sensitized with different amounts of these particles were measured, in cylindrical charges, by ionization pins and optical fibers. The detonation velocity of emulsion explosives shows a non-monotonic evolution with the density with the maximum being reached far below the maximum density. The detonation fails when the density approaches the one of the matrix. The failure diameter increases with increasing density. For low densities the detonation velocity is almost independent of the charge diameter and it is close to the values predict by BKW EoS. The effect of the nature and size of the microbubbles on the detonation front curvature and failure diameter was also determined.

2:30PM K5.00004 Carbon solids in oxygen-deficient explosives (LA-UR-13-21151)³, TRAVIS PEERY. Theoretical Division, Los Alamos National Laboratory — The phase behavior of excess carbon in oxygen-deficient explosives has a significant effect on detonation properties and product equations of state. Mixtures of fuel oil in ammonium nitrate (ANFO) above a stoichiometric ratio demonstrate that even small amounts of graphite, on the order of 5% by mole fraction, can substantially alter the Chapman-Jouguet (CJ) state properties, a central ingredient in modeling the products equation of state. Similar effects can be seen for Composition B, which borders the carbon phase boundary between graphite and diamond. Nano-diamond formation adds complexity to the product modeling because of surface adsorption effects. I will discuss these carbon phase issues in our equation of state modeling of detonation products, including our statistical mechanics description of carbon clustering and surface chemistry to properly treat solid carbon formation.

This work is supported by the Advanced Simulation and Computing Program, under the NNSA.

2:45PM K5.00005 Pressure waves generated by metastable intermolecular composites in an aqueous environment¹, GEORGE MAINES, MATEI RADULESCU, ANTOINE BACCIOCHINI, BERTRAND JODOIN, University of Ottawa, JULIAN LEE, DRDC-Suffield — In the present study, pressure waves generated by a metastable intermolecular composite (MIC) have been measured experimentally in an aqueous environment. Experiments were performed in a 1.0 L high pressure chamber mounted with high resolution pressure transducers and designed with optical access. Samples consisting of a stoichiometric mixture of aluminum and copper(II)oxide particles were evaluated. Two types of samples were constructed; a mixture of micron-sized raw powders, and ball milled powders with a lamellated nanostructure. A planetary mill was used to refine reactant powders from micron- to nano-scale dimensions. Manual compaction and cold spray deposition techniques were used to consolidate powders in various densities. The dynamics of the pressure wave and high pressure gas bubble were monitored via pressure data and high-speed Schlieren visualization. The effects of reactant particle size and sample density have been evaluated quantitatively and compared with equilibrium calculations. Dynamics of the pressure wave were correlated with the amount of gas released and the rate of burning of the sample material.

¹Work supported by DRDC Suffield (Dr. Julian J. Lee)

3:00PM K5.00006 Nano-Scale Energetic Films by Superfluid Helium Droplet Assembly, SAMUEL EMERY, Air Force Research Laboratory, JASON BOYLE, Naval Surface Warfare Center Indian Head Division, KEITH RIDER, Longwood University, BRIAN LITTLE, C. MICHAEL LINDSAY, AMANDA SCHRAND, Air Force Research Laboratory — We have recently transitioned superfluid helium droplet assembly of clusters into a deposition tool that is capable of creating nano-structured films of composite metal-based energetic materials (EM). Such materials are ideal candidates to study propagation of reactions at small scale, and could be alternatives to organic based EM due to their higher energy densities. The helium droplet methodology may also provide a solution overcoming issues of reaction-limiting effects such as the formation of oxide layers by exploiting ‘magic-number’ cluster sizes and core-shell cluster mechanisms. This presentation will describe the following: foundational work to model and characterize the deposition of magnesium clusters by superfluid helium droplet assembly, our efforts to produce magnesium-Fomblin core-shell EM cluster-based films on a surface, and our early attempts at making intermetallic cluster-based films.

Tuesday, July 9, 2013 1:45PM - 3:15PM –
Session K6 EM.1 Shock to Detonation II
Cascade II - Dana Dettelbaum, Los Alamos National Laboratory

1:45PM K6.00001 Shock-to-detonation transition of RDX and NTO based high explosives: experiments and modeling, GERARD BAUDIN, MARIE ROUDOT, MARC GENETIER, CEA DAM Gramat — Composite HMX and NTO based high explosives (HE) are widely used in ammunitions. Designing modern warheads needs robust and reliable models to compute shock ignition and detonation propagation inside HE. Comparing to a pressed HE, a composite HE is not porous and the hot-spots are mainly located at the grain–binder interface leading to a different behavior during shock-to-detonation transition. An investigation of how shock-to-detonation transition occurs inside composite HE containing RDX and NTO is proposed in this lecture. Two composite HE have been studied. The first one is HMX – NTO – HTPB 12:72:16. These HE have been submitted to plane sustained shock waves at different pressure levels using a laboratory powder gun. Pressure signals are measured using manganin gauges inserted at several distances inside HE. The corresponding run-distances to detonation are determined with optical access. Samples consisting of a stoichiometric mixture of aluminum and copper(II)oxide particles were evaluated. Two types of samples were constructed; a mixture of micron-sized raw powders, and ball milled powders with a lamellated nanostructure. A planetary mill was used to refine reactant powders from micron- to nano-scale dimensions. Manual compaction and cold spray deposition techniques were used to consolidate powders in various densities. The dynamics of the pressure wave and high pressure gas bubble were monitored via pressure data and high-speed Schlieren visualization. The effects of reactant particle size and sample density have been evaluated quantitatively and compared with equilibrium calculations. Dynamics of the pressure wave were correlated with the amount of gas released and the rate of burning of the sample material.

2:00PM K6.00002 ABSTRACT WITHDRAWN

2:15PM K6.00003 Shock Initiation Experiments with Ignition and Growth Modeling on Low Density HMX, FRANK GARCIA, KEVIN S. VANDERSALL, CRAIG M. TARVER, Lawrence Livermore National Laboratory — Shock initiation experiments on low density (1.24 and 1.64 g/cm³) HMX were performed to obtain in-situ pressure gauge data, characterize the run-distance-to-detonation behavior, and provide a basis for Ignition and Growth reactive flow modeling. A 101 mm diameter gas gun was utilized to initiate the explosive charges with manganin piecezoresistive pressure gauge packages placed between packed layers (1.24 g/cm³) or sample disks pressed to low density (1.64 g/cm³). The measured shock sensitivity of the 1.24 g/cm³ HMX was similar to that previously measured by Dick and Sheffield et. al. and the 1.64 g/cm³ HMX was measured to be much less shock sensitive. Ignition and Growth model parameters were derived that yielded good agreement with the experimental data at both initial densities. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
Tuesday, July 9, 2013 1:45PM - 3:15PM – Session K7 ME.4 Strength V Grand Crescent - Justin Brown, Sandia National Laboratories

1:45PM K7.00001 The effect of microstructure on Rayleigh-Taylor instability growth in solids, Russell Olsson, Los Alamos National Laboratory — The effect that grain size and material processing have on high-strain rate deformation of copper and tantalum has been assessed through measurements of unstable Rayleigh-Taylor (RT) perturbation growth. The dynamic loading conditions and initial sinusoidal perturbations imposed on the samples are kept constant while the microstructure of the sample material is varied. Different polycrystalline grain-sizes, single-crystal orientations, and strain-hardened samples have all been dynamically tested. The RT perturbation growth is measured by acquiring a time-sequence of radiographs using the Los Alamos National Laboratory Proton Radiography (pRad) Facility. Single-crystal orientation and stain hardening due to material processing are both observed to affect the perturbation growth. However, polycrystalline grain size variations in both tantalum and copper samples do not affect the RT perturbation growth.

In collaboration with Ellen Cerreta, Christopher Morris, Russell Olson, Dean Preston, Joseph Stone, Dale Tupa, and Wendy Vogan-McNeil, Los Alamos National Laboratory.

2:15PM K7.00002 Explosively driven two-shockwave tools with application to ejecta formation at the Los Alamos National Laboratory Proton Radiography Facility, William Buttlar, Los Alamos National Laboratory — We present the development of an explosively driven physics tool to generate two mostly uniaxial shockwaves. The tool is being used to extend single shockwave ejecta models to a subsequent shockwave event separated by a time interval on the order of a few microseconds. We explore the possibility of varying the amplitude of both the first and second shockwaves, and we apply the tool in experimental geometries on Sn with a surface roughness of $R_a = 0.8 \mu m$. We then evaluate the tool further at the Los Alamos National Laboratory Proton Radiography (pRad) Facility in an application to Sn with larger scale perturbations of wavelength $550 \mu m$, and various amplitudes that gave wave-number amplitude products of $\kappa_2 k / \lambda = (3/4, 1/2, 1/4, 1/8)$, where the perturbation growth in each case is $\kappa = 2\pi / \lambda$. The pRad data and velocimetry imply it should be possible to develop a second shock ejecta model based on unstable Richtmyer-Meshkov physics.


2:45PM K7.00003 Measurement of the Response of an Elastomer at Pressures Up to 9GPa and Strain Rates of $10^5$ to $10^6 s^{-1}$, Tong Jiao, Rodney Clifton, Brown University — Pressure-shear plate impact (P SPI) experiments have been conducted to study the mechanical response of an elastomer at high pressures and high strain rates. The previously determined isentrope has been extended to 9 GPa. At this pressure, the high-strain-rate shearing resistance of polyurea is approximately 500MPa-comparable to, or greater than, that of high strength steels and at much lower weight. It was also found that polyurea exhibits remarkable “recoil” during unloading from these high pressures. A new symmetric pressure-shear plate impact (SPSPI) configuration has been developed in order to enable the direct measurement of the thickness-averaged nominal strain rates of the sample – as well as the tractions on both of its interfaces with linear elastic plates. This enhancement is made possible by using a symmetric configuration for which the velocity of the mid-plane of the sample is known from symmetry to be one-half of the impact velocity. One-dimensional elastic wave theory is used to obtain tractions and particle velocities at the sample/anvil interface from the measured rear-surface velocities. In this way, nominal strain-rate histories are obtained for both longitudinal and shear strains.
3:00PM L1.00004 Preheating study by VISAR measurements in laser-driven shocks on SGII facility1, XIUGUANG HUANG, Professor, HUA SHU, Assistant Professor, SIZU FU, Professor, JUNJIAN YE, Associate Professor, ZHIHEN FANG, GUO JIA, ZHIYONG XIE, HUAZHEN ZHU, Assistant Professor, TAO WANG, None, SHANGHAI INSTITUTE OF LASER PLASMA TEAM — The preheating of laser-irradiated aluminum planar or multi-step targets has been measured by velocity interferometer system for any reflector (VISAR), which detects the target's rear surface motion prior to shock wave breakout. The preheating temperature was induced from the linear expansion theory and release isentropic data, respectively. And the results calculated from both methods are consistent. The results also show that the preheating temperature decreases nearly linearly with decreasing laser energy or increasing foil's thickness. Moreover, the preheating effects drop sharply by only burning a thin high-Z layer (~1.5µm Au) in the aluminum foil. Base on above results and other results from X-ray crystal spectrometer, electron energy spectrometer, and our analytical calculation, we think that the source of preheating is mainly of hard X-ray.

1Shanghai Institute of Laser Plasma

Tuesday, July 9, 2013 3:30PM - 5:30PM
Session L1 ME.3 Inelastic Deformation, Fracture, and Spall III Grand Ballroom I - Satish Gupta, Bahba Atomic Research Center

3:30PM L1.00001 Experimental observation and theoretical modeling of the effect of magnetic field on the strength of molybdenum under ramp wave compression1, JOW DING, Washington State University, C. SCOTT ALEXANDER, JAMES ASAY, Sandia National Laboratories — A new experimental technique has been developed at Sandia National Labs to study the dynamic material strength at high pressures using "magnetically applied pressure shear (MAPS)" ramp waves. In order to apply sufficient shear traction to the test sample, the driver must have substantial strength. Molybdenum was selected for this reason along with its good electrical conductivity. It was observed that an imposed magnetic field of around 10 Tesla induced some annealing on molybdenum. Furthermore, when subjected directly to magnetohydrodynamic loading as encountered for the driver material, molybdenum exhibited an apparently stiff response and did not show a discernible elastic plastic transition. To better understand the experiments and establish a predictive capability for molybdenum, a tentative strength model that incorporates the possible magnetic effects including magnetic diffusion, Joule heating, and the coupling between the magnetic field and material strength has been developed. Experimental observations and the model will be discussed.

1Sandia National Labs is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Dept. of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

3:45PM L1.00002 Elastic-Plastic Deformation of Molybdenum Single Crystals Shocked along <100> , ANIRBAN MANDAL, Y.M. GUPTA, Washington State University — To examine and understand elastic-plastic deformation in shocked Molybdenum (Mo), single crystal samples (99.99% purity) were shocked along <100> orientation. The peak longitudinal stress in our experiments was ~12 GPa and sample thicknesses ranged between 0.23 and 2.3 mm. The Mo samples were backed by c-axis sapphire optical windows, and wave profiles were measured at the Mo/sapphire interface using laser interferometry (VISAR). A two-wave structure, expected from elastic-plastic deformation, was observed in all cases. Elastic wave amplitudes ranged between 2.9 and 4.2 GPa with an average value of 3.6 GPa. The scattered observed in the elastic wave amplitudes, though somewhat high, is comparable to that observed in a previous work on single crystals of tungsten, another bcc metal (T. E. Michaels, Ph. D. thesis, WSU). Measured wave profiles showed stress relaxation behind the elastic wave front for samples of 0.46 mm or larger in thickness. No obvious correlation could be established between the measured elastic wave amplitudes and the sample thicknesses examined. Relationship of the present results to slip systems postulated for Mo will be discussed.

This work is supported by DOE/NNSA.

4:00PM L1.00003 Effect of shock wave duration on dynamic failure of Tungsten Heavy Alloy , CARL P. TRUJILLO, E. PABLO ESCOBEDO, ERIC N. BROWN, ELLEN K. CERRERA, GEORGE T. GRAY, Los Alamos National Laboratory — It has been well established that dynamic fracture or spall is a complex process strongly influenced by both microstructure and the loading profile imparted to the specimen. Having previously considered ductile materials with damage and deformation kinetics that are slow relative to the shock wave, here we consider a brittle material with large damage and deformation kinetics that are fast relative to the shock wave. The present study elucidates the effect of loading profile on the fundamental mechanisms of brittle fracture in brittle tungsten heavy alloy (WHA) specimens. Spall experiments are performed on two significantly distinct shock pulse durations and accompanying unloading rates. Detailed fractographic analyses of the damage in the spalled WHA samples as a function of shock-wave profile of comparable peak stress is presented. For both profiles, it is observed that the failure in WHA is by brittle trans-particle crack growth with additional energy dissipation through crack branching in the more brittle tungsten particles. We also observe that for the 15.4 GPa peak shock stress, the wave profile does not influence the spall strength significantly. This is believed to be directly linked with the relative insensitivity of WHA to time dependent processes.

4:15PM L1.00004 Study of leading features at shock-loading and further unloading , ALEXEY FEDOROV, ANATOLY MIKHAILOV, STANISLAV FINYUSHIN, DMITRY NAZAROV, EVGENY CHUDAKOV, DENIS KALASHNIKOV, EVGENY BUTUSOV, None — The determination of mass, size, shape and velocity of particles, which appear as a result of microcumulative ejection from the metal surface at the moment of shock wave outlet, is a very complicated and multivariate problem. The presentation object is to value lead melting area boundaries and to measure velocity of particle cloud ejected from the surface under shock loading. The free surface and ejecting particle cloud velocities were simultaneously measured at the moment of shock wave outlet, is a very complicated and multivariate problem. The presentation object is to value lead melting area boundaries and to measure velocity of particle cloud ejected from the surface under shock loading. The free surface and ejecting particle cloud velocities were simultaneously measured at the moment of shock wave outlet. The material seems to be in the composite state (liquid-solid phase) at the pressure of 22 GPa and more, the preheating temperature decreases nearly linearly with decreasing laser energy or increasing foil's thickness. Moreover, the preheating effects drop sharply by only burning a thin high-Z layer (~1.5µm Au) in the aluminum foil. Base on above results and other results from X-ray crystal spectrometer, electron energy spectrometer, and our analytical calculation, we think that the source of preheating is mainly of hard X-ray.

The free surface and ejecting particle cloud velocities were simultaneously measured at the moment of shock wave outlet. The material seems to be in the composite state (liquid-solid phase) at the pressure of 22 GPa and more, the preheating temperature decreases nearly linearly with decreasing laser energy or increasing foil's thickness. Moreover, the preheating effects drop sharply by only burning a thin high-Z layer (~1.5µm Au) in the aluminum foil. Base on above results and other results from X-ray crystal spectrometer, electron energy spectrometer, and our analytical calculation, we think that the source of preheating is mainly of hard X-ray.

4:30PM L1.00005 Influence of preliminary loading on formation of adiabatic localized shift in copper , VICTOR PUSHKOV, ALEXEY YURLOV, ALEXEY PODURETS, ANDREW TSIBIKOV, Russian Federal Nuclear Center - VNIIEF, CONSTANTINE NOVIKOV, Russian Federal Nuclear Center - VNIIEF, MAXIM PUKHOV, Russian Federal Nuclear Center - VNIIEF — It is revealed (for example, by G.T.Gray and co-workers) that formation of strain localization centers is very sensitive to the initial density of defects and peculiarities of the basic microstructure. At the same time, the other experts revealed in their works that the material ability for strain hardening plays an important role in localization of shear bands. Presently this process is still under active study. This paper is devoted to results of investigation of localized shift in as-received copper, and which was subjected to preliminary quasi-isentropic shock loading by the pressure of ~30 GPa. Tests were performed with hat-shaped samples by the SHPB method. The authors present estimation of quantitative characteristics of localized shift in tested materials (shear stress, relative shear strain, shear band width, relative strain rate in shear band). The paper includes data of metallographic investigations of the tested samples. Also the authors made an attempt of numerical simulation of stress field change during formation.
4:45PM L1.00006 The Spall Strength and Hugoniot Elastic Limit of Monocrystalline and Polycrystalline Copper near Melting Temperature, SERGEY RAZORENOV, Institute of Problems of Chemical Physics RAS, Russia, EUGENY ZARETSKY, Ben Gurion University of the Negev, Israel, ANDREY SAVINYKH, Institute of Problems of Chemical Physics RAS, Russia — In the present work the Hugoniot elastic limit (HEL) and the spall strength of the polycrystalline commercial grade copper and of the copper single crystal of [100] and [111] orientations were determined for the sample temperatures varying from 293 to 1353K, what is some 3K below the copper melting point Tm. The preheated samples in thickness between 0.5 and 2 mm were shock-loaded by the copper plates of 1-mm thickness accelerated up to 300-400-m/s velocity in the 58-mm smooth bore gas gun, or by the aluminum plates of 0.4 mm in thickness accelerated up to ~660 m/s with explosive facilities. The velocity histories of the free rear surface of the loaded samples were recorded with VISAR laser velocimeter. The velocity histories of the samples of polycrystalline copper demonstrate 9-fold growth of the stress at HEL between room and melting temperatures. Unlike the other metals, commercial grade copper maintains a very high spall strength near melting point; it is only twice as low as that of the copper at 0.85 Tm. The copper single crystals of the both orientations also demonstrate substantial spall strength at 0.94 Tm (1273K). But the increase of the stress at HEL with temperature in these samples is much weaker than that found for polycrystalline samples of copper.

5:00PM L1.00007 Ductile damage in Taylor and Rod-on-rod impact experiment, GIANLUCA IANNITTI, Techdyn Engineering, ANDREW RUGGIERO, NICOLA BONORA, DOMENICO GENTILE, University of Cassino and Southern Lazio — At equivalent impact velocity, pressure in Taylor and ROR impact experiment is not the same and this reflects in the resulting condition for ductile damage development. In this work, finite element parametric simulation was performed to investigate pressure wave development as a function of material and target work hardening curve. Using the Bonora damage model, the impact velocity necessary for generating ductile damage in high purity copper was assessed. Taylor and ROR experiments were performed at different equivalent impact velocities and metallographic investigation were performed on impacted samples in order to validate damage model predictions. In addition, the effect of temperature on damage development was also investigated performing impact tests at different reference temperatures.

Tuesday, July 9, 2013 3:30PM - 5:30PM –
Session L2 HM High Energy Density Materials I Grand Ballroom II - Gilbert Collins, Lawrence Livermore National Laboratory

3:30PM L2.00001 Ramp Compression of materials to high-pressure low-temperature states, RAYMOND SMITH, Lawrence Livermore National Laboratory — The thermodynamics of compression are typically examined under isothermal conditions or with shock waves, where compressions are limited by the achievable pressure or dissipative heating, respectively. A relatively new dynamic compression technique, ramp compression, enables the adiabatic compression of matter with reduced dissipative heating as compared to shock compression and potentially allows the exploration of solids to the extreme densities expected to exist in the deepest interiors of giant planets. Ramp compression is however unstable relative to a shock because sound velocities typically increase with pressure. Therefore, to ramp compress matter into the multi-Mbar pressure regime, the pressure-loading history must be gentle enough to avoid shock formation, while sufficiently intense to achieve high pressures, constraints that until now were out of reach for laboratory experiments. I will describe ramp compression experiments on the NIF laser in which the stress-density of diamond and Fe were determined to peak pressures of 50Mbar and 8Mbar, respectively. I will also present preliminary data from the new NIF x-ray diffraction platform.

4:00PM L2.00002 Strongly Coupled Plasma Shock Compression, VLADIMIR FORTOV, Joint Institute for High Temperature, Russian Academy of Sciences — The behavior of matter at extremely high pressures is of high principal interest for understanding the structure and evolution of astrophysical objects and many energy, nuclear and chemical technologies. Dynamics methods of generation of extremely high pressures in dense plasma, based on the compression and nonreversible heating of matter in intensive shock waves and waves of adiabatic discharge, are considered. To generate shock waves in the megabar pressure range the cylindrical and spherical condensed high explosives, laser and corpuscular beams, high velocity impacts, and soft X-rays were used. The highly time-resolved diagnostics of the extreme states of plasma were carried out with differential laser indicators of velocity, fast acting electron-optical transducers, pyrometers, and high-speed spectrometers equipped with the electron-optical transmission lines. The experimental data obtained and the physical models of behavior of plasma at extremely high pressures, temperatures and deformation rates are discussed. These are the metallization and dielectrization of strongly compressed matter, high temperature thermodynamics and phase transitions, deformation of energy spectrum of compressed atoms and strength and elastic-plastic phenomena, kinetics of phase transitions. We analyzed the shear viscosity of matter as an indicator of particles correlations in a broad region of parameters from Plank’s scale to laboratory conditions. Wide-range semi-empirical equations of state and models are constructed, which were used for multidimensional numerical simulation of pulsed high-energy processes.

4:30PM L2.00003 Structure Measurements of Highly Compressed Aluminum using X-Ray Thomson Scattering, TAMMY MA, Lawrence Livermore National Laboratory — X-ray Thomson scattering (XRTS) is a powerful technique to characterize materials in the challenging warm dense matter regime. In addition, XRTS measurements enable the benchmarking of dense plasma models and provide validation for EOS. Spectrally, angularly, and temporally resolved XRTS has been used to probe highly compressed aluminum (3x solid density) with 18 keV x-rays. The measured elastic scattering feature shows a well-pronounced correlation characteristic of the warm dense matter state. For the first time, the measurements of the scattering are precise enough to distinguish between theoretical models for the ion structure and show that screening effects must be accounted for in order to fit the shape and absolute intensity of the data. This further demonstrates the capability of XRTS to resolve the ion-ion correlation for an accurate measurement of compression. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
5:00PM L2.00004 X-ray Thomson scattering of warm dense matter on the Z-accelerator

5:15PM L2.00005 Cylindrically Convergent Implosions of Metal Liners for Driving an Isentropic Compression in Cryogenic Deuterium

Tuesday, July 9, 2013 3:30PM - 5:30PM –
Session L3 NT.2 Novel Techniques: Temperature
Fifth Avenue - Shawn McGrane, Los Alamos National Laboratory

3:30PM L3.00001 Thermal imaging of Al-CuO thermites

3:45PM L3.00002 Er,Yb:ZrO₂ / Eu₂O₃ Core/Shell Assemblies as Potential Temperature Sensors in Explosions

4:00PM L3.00003 Flash lamp integrating sphere technique for measuring the dynamic reflectance of shocked materials
4:30PM L3.00004 Optical reflectance as a dynamic temperature diagnostic, DANIEL DOLAN, CHRISTOPHER SEAGLE, TOM AO, Sandia National Laboratories — Reliable temperature measurements of materials under dynamic compression remain elusive, especially in quasi-isentropic experiments. Optical pyrometry with nanosecond time resolution is essentially impossible for samples below 1000 K—not enough photons are emitted to make measurable temperature measurements. Rather than relying on light emission from the sample, one can also infer temperature by the light reflected by the sample. Thermoreflectance measurements are a proven technique in static systems and can readily be applied to dynamic compression experiments. Gold is an ideal candidate for dynamic thermoreflectance measurements. Gold coatings rapidly equilibrate with their surroundings, acting as an embedded gauge that can be probed optically. The optical properties of gold vary in the visible spectrum, and these variations are known to change with temperature, so in principle one can infer temperature from time-resolved reflectivity measurements. Calibration is the largest barrier for using embedded gold gauges because both temperature and pressure contribute to the measurement. This presentation will discuss static and dynamic calibration efforts to establish gold as a dynamic thermoreflectance standard.

1 Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85

4:45PM L3.00005 Probing Shock Compressed Silicon Metallization using VIS/NIR Reflectivity, SUZANNE ALI, Univ. of California, Berkeley, CYNTHIA BOLME, Los Alamos National Lab, RAYMOND JEANLOZ, Univ. of California, Berkeley, GILBERT COLLINS, Lawrence Livermore National Lab — Broadband reflectivity measurements provide detailed information about the optical and electronic properties of shocked matter, complementing other spectroscopic techniques and increasing the accuracy of pyrometric measurements, which is vital for improving models of planetary cores. A time resolved broadband VIS/NIR reflectivity diagnostic was constructed and used to observe the metallization of shock compressed single crystal <111> silicon at Jupiter Laser Facility at Lawrence Livermore National Lab. A 50-100 fs 800 nm pulse was first sent through a pulse stacker and then an intense white light pulse with wavelengths from ~400 nm to ~1200 nm was generated by focusing the stacked pulses into a water cell. The white light pulses were then sent into the chamber and reflected from the target surface. The reflected light was dispersed using a custom spectrometer which was coupled to a streak camera. On transition to the β-Sn phase a dramatic increase in reflectivity was observed in the NIR, and to a lesser extent in the visible. This is congruent with the decrease in resistivity that accompanies closure of the silicon band gap and metallization.

5:00PM L3.00006 Application of Heterodyne Velocimetry and Pyrometry as Diagnostics for Explosive Characterisation, JAMES FERGUSON, PETER TAYLOR, Hydrodynamics Department, AWE, Aldermaston, Reading, Berkshire, RG7 4PR, UK — The results of four cylinder tests performed on two batches of an HMX based explosive using a new suite of diagnostics are described. Heterodyne laser velocimetry (hEtV) and pyrometry were fielded for the first time on cylinder tests within AWE. Pyrometry gave a measurement of the temperature of the detonating HE of 2600-3000 K. Sixteen channels of hEtV were fielded and provided high fidelity expansion data at distances of up to 30 m. High speed framing camera images were obtained and show no signs of cylinder break up or spalling until distances greater than 35 mm. The expansion data has revealed the elastic pre-cursor in the cylinder wall and made it possible to resolve up to 8 shock reverberations in the wall as it expands. The expansion of the cylinder wall was recorded both before and after steady state detonation has been reached and the results compared. hEtV probes were fielded at different angles to the expanding cylinder wall allowing both the vertical and horizontal expansion velocity to be determined. The extra information that these cylinder tests yielded will allow for more accurate code validation and determination of the equation of state.

1 Hydrodynamics Department, AWE, Aldermaston, Reading, Berkshire, RG7 4PR, UK

5:15PM L3.00007 Pyrometric temperature measurements of shocked metals with uncertainties of less than 2%, BRANDON LALONE, GERALD STEVENS, WILLIAM TURLEY, National Security Technologies, Special Technologies Laboratory, DAVID HOLT KAMP, Los Alamos National Laboratory, ADAM IVERSON, ROBERT HIXSON, LYNN VEESER, National Security Technologies, Los Alamos Operations — Advances in reflectance measurements have enabled accurate measurements of the emissivity of metals subjected to shock wave compression. Using three spectral bands, we performed reflectance and radiance measurements of shock compressed tin glued to LiF windows and combined them to determine time resolved temperatures with uncertainties of less than 2%. Details of the uncertainty analysis are discussed. The tin samples were shock loaded using high explosives so there is a Taylor wave stress release that follows the shock front. Stress histories of the release were determined from PDV measurements and were combined with the temperatures to obtain temperature-stress release paths for the tin-glue-LiF interface. We discuss the link between the experimental release paths and release isentropes that begin on the principal shock Hugoniot. There is a complex relationship between the measured interface temperatures and the temperatures within the interior of the samples which complicates the analysis. Several of the complications are briefly discussed and interior temperatures are estimated. This work was done by National Security Technologies, LLC, under Contract No. DE-AC52-06NA25946 with the U.S. Department of Energy, and supported by the Site-Directed Research and Development Program.

Tuesday, July 9, 2013 3:30PM - 5:15PM – Session L4 NM.3 Novel Properties I Vashon - Richard Kaner, University of California, Los Angeles

3:30PM L4.00001 Phase stability and Transitions’ mechanisms in MPO4 compounds under high pressures, SURINDER M. SHARMA, Bhabha Atomic Research Centre, Mumbai, India — MPO4 (M = Al, Ga, In, B) compounds exist in several tetrahedrally connected structures at ambient conditions. Our experimental and theoretical investigations show that pressure brings about systematic changes in the nature of polyhedral coordination. Unlike the structural analog SiO2 most of MPO4 compounds evolve through an intermediate Cmcm phase before transforming to still denser phases in which even phosphorus is also octahedrally coordinated. Our investigations also reveal that over-pressure helps bypass the region of co-existence of parent and daughter phases implying a barrierless path for emergence of higher coordinated states. Results of several investigations have helped obtain a unified understanding of these compounds and will be presented.

4:00PM L4.00002 Molecular Routes Syntheses of Nano-structured C and C-N Compounds in High Pressure and Temperature using LH-DAC, KEN NIWA, MASASHI HASEGAWA, TAISHI HORIBE, YUKI JIN, KEIJI KUSABA, Nagoya University, KEISUKE YASUDA, RYOYA ISHIGAMI, Wakasa-wan Energy Research Center — Molecular routes syntheses in high pressure and temperature are powerful to obtain novel materials, especially carbon-based inorganic compounds. We have tried to synthesize new nano-structured C and C-N inorganic compounds from heterocyclic compounds in high pressure and temperature using a Laser-Heated Diamond-Anvil Cell (LH-DAC) system and characterized by XRD, SEM-EDX, TEM-EELS, Raman, IRS and ERDA. Some heterocyclic organic compounds were reacted to various kinds of nano-structured carbons such as nano-diamonds, carbon nano-tubes and carbon nano-cones. We have also synthesized graphite-like nano-structured C-N compounds using this technique. They showed petal-like morphology similar to “carbon nano-wall”. The thickness of petals was several tens of nm. Petals were found to have a graphite-like layer structure on the basis of TEM experiments. It was found that the c-axis lattice constant changes almost linearly as a function of the analyzed nitrogen content. We will also report synthesis results of nano-structured C-N compounds using GPa-range supercritical fluid in DAC.
A new hexagonal carbon nitride synthesized at high pressure and high temperature

4:15PM L4.00003 A new hexagonal carbon nitride synthesized at high pressure and high temperature, MASAYA SOUGAWA, YUTA SHIMA, MASAAKI HIRAI, KENICHI TAKARABE, Okayama University of Science, TAKU OKADA, The Institute for Solid State Physics, University of Tokyo, THE INSTITUTE FOR SOLID STATE PHYSICS, UNIVERSITY OF TOKYO COLLABORATION — A new hexagonal carbon nitride has been synthesized by subjecting the C₃N₄H₄ precursor to high pressure and high temperature. The XRD pattern of the new hexagonal carbon nitride is indexed as the hexagonal unit cell with the lattice parameters; \( a = b = 2.83 \text{ Å}, c = 9.82 \text{ Å} \) (\( V \approx 68.10 \text{ Å}^3 \)). The unit cell of this new hexagonal carbon nitride differs from the several hexagonal carbon nitrides reported so far by the theoretical and experimental studies. Hart et al. proposed the hexagonal structure with 1:1 stoichiometry is based on the known GaSe layer. The space group is \( P6_3/mmc \). Bjojdys et al. synthesized the graphitic-C₃N₄ \( (g-C_3N_4) \) with the hexagonal unit cell with the lattice parameters \( a = 6.43 \text{ Å}, c = 6.72 \text{ Å} \) (\( V \approx 414.09 \text{ Å}^3 \)), and the space group is \( P6_3/cm \). These reported hexagonal lattice constants disagree with the new hexagonal carbon nitride synthesized in this report. We will report the full analysis of the crystal structure of the new hexagonal carbon nitride at the conference.

4:30PM L4.00004 High-Pressure Induced New Phases and Properties in Typical Molecular Systems, TIAN CUI, State Key Lab of Superhard Materials, College of Physics, Jilin University — High pressure introduces new phases by the rearrangement of atoms and reconfigurations of electronic states in materials, often with new physical and chemical phenomena. Study of the new phases in typical molecular systems under high pressure is an interesting subject, such as energy storage materials of solid hydrogen and polymeric nitrogen, hydrogen-rich compound with high-Tc superconductivity under high pressure, high pressure induced metallization of hydrogen, etc. High-pressure structures and pressure-induced phase transitions in the typical molecular solids, such as solid iodine, CHBr₃, N₂/CN, HBr/HCl, hydrogen-rich compounds (H₂S, ZrH₂, AsH₃, BaReH₉, etc.), and group iva hydrides (Si2H6, Ge2H6, Sn2H6, etc.) are investigated extensively by means of first-principles density functional theory and extensive prediction strategies. We focus on the structural and electronic properties of the confined species inside the 1D channel of AFI under pressure. The pronounced pressure-induced prolongation of molecular chains, pressure-induced rotation of the confined neutral molecules, and the abrupt transition in the vibrational frequency of the confined iodine due to the change of the interaction between the confined species and host wall have been observed.

Tuesday, July 9, 2013 3:30PM - 5:30PM
Session L5 GP1: Geophysics III  Cascade I - Zsolt Jenei, Lawrence Livermore National Laboratory

3:30PM L5.00001 Pressure-induced structural change in molten basalt. CHRysteLESanLOUp, James DREWITT, PHILLIP DALLADAY-SIMPSON, DONNA MORTON, University of Edinburgh, NACHIKETA RAI, VU University, Amsterdam, ZUZANA KONOP-KOVA, DESY, Hamburg, WIM VAN WESTREHEN, VU University, Amsterdam, WOLFGANG MORGROEN, DESY, Hamburg — Magmas are produced at depth in the Earth, and occurrences of their presence at greater depths are reported based on seismological information, such as the 410 discontinuity or atop the core-mantle boundary. Understanding the presence and eventual stability of magmas in the deep mantle requires a knowledge of their physical properties. However, this has been impeded for a long time due to the challenging nature of the experiments. In the recent years, structural and density information on silicate glass have been obtained up to record pressures of up to 100 GPa, a first major step towards obtaining data on the molten state. Here, the structure of molten basalt is reported up to 60 GPa by means of in situ x-ray diffraction, and structural changes are evidenced. Silicon coordination increases from 4 at ambient conditions to 6 at 35 GPa, similarly to what has been reported in silica glass. Compressibility of the melt above completion of Si coordination change is lower than at lower pressure \( (P) \) conditions, implying that a single equation of state can not accurately describe density evolution of silicate melts over the whole mantle \( P \)-range. It also implies that melts can be buoyantly stable circa 35-40

3:45PM L5.00002 Ultrafast x-ray studies on the dynamics of structural transitions in amorphous and crystalline SiO2. ARIANNA GLEASON, Stanford University, CINDY BOLME, Los Alamos National Lab, WENDY MAO, Stanford University, WENGE YANG, Advanced Photon Source, Argonne National Lab, HAe JA LEE, BOB NAGLER, ERIC GALTIER, DESPINA MILATHIANAKI, SLAC, LCLS, RICHARD SANDBERG, Los Alamos National Lab — Silica (SiO2) and its phase transitions at high pressure and temperature are of paramount importance to geophysics as it is the dominant chemical constituent of the Earth’s mantle. Knowledge of its properties and behavior under pressure is essential to interpretation of seismic studies, high velocity cratering impact events, and to understanding the dynamics and evolution of the terrestrial planetary interiors. Here we present unprecedented experimental results on the phase transition kinetics of amorphous and crystalline SiO2 with sub-nanosecond resolution. These novel experiments, performed at LCLS, SLAC are the first ever measurements of a non-metal showing transitions from amorphous SiO₂ to polycrystalline coesite and/or stishovite. X-ray diffraction patterns were collected with varied time delays and optical laser powers to achieve a wide sampling of pressure-temperature-time-phase space. Our datasets include information on time-resolved phase growth, grain size and texture development/evolution.

4:00PM L5.00003 Dynamic dehydration processes of porous antigorite by impact. TOSHIMORI SEKINE, TOMOAKI KIMURA, Hiroshima University, TUTOMU MASHIMO, Kumamoto University, TAKAMICHI KOBAYASHI, National Institute for Materials Science — Antigorite Hugoniot indicates that it is stable up to a pressure of ~50 GPa. When antigorite is under a circumstance surrounding pores in natural meteorite, the stability may change with local temperature and pressure. Antigorite acts as a potential carrier of water in the solar system, the dynamic dehydration process is a key to understand the ability of carrier. We carried out shock recovery experiments in a pressure range between 5 GPa and 60 GPa. The recovered samples were investigated using XRD, TEM, and TG-DTA. In order to recover samples, it was found that the amount of sample was critical. There seems to be two steps of dehydration processes; limited dehydration below 20 GPa and violent dehydrations above 20 GPa. The violent reaction depends on the porosity of a sample. The TG-DTA results coupled with XRD indicate that dehydration products are forsterite and enstatite without their high-pressure forms and hydrous minerals. The amount of amorphous phase was only a trace based on the TEM observations, implying that dehydration reaction may have occurred at high temperatures for the crystals to grow during pressure release.
These hydrogen-rich materials with nontraditional stoichiometries are computed to undergo an insulator to metal transition at pressures attainable in diamond. The stabilization pressure to the ionization potential, and the nature of the hydrogenic sublattice to the strength of the metal-hydride interaction can be made. The H\(^{-}\)\(+\) ratio, M\(\text{XtalOpt}\), an open-source evolutionary algorithm for crystal structure prediction. Whereas at 1 atmosphere the classic alkali hydrides combine in a one-to-one intuition (developed at 1 atmosphere) would be exceedingly difficult, making automated structure search techniques prudent. For this reason, we have written or stoichiometries, and unexpected electronic structures may be achieved by applying external pressure. The prediction of these structures using our chemical Polyhydrides and Subhydrides

5:00PM L5.00006 Deformation response of rocky material for a range of stress states and strain rates , ANGELA STICKLE, K.T. RAMESH, The Johns Hopkins University — The failure of rocky materials under impact conditions will occur in a rapidly evolving, multi-axial stress state. Significant improvements in understanding impact processes, then, can come from physically-based models for the dynamic response of materials under general stress states. To provide insight into the deformation response of geologic materials under impact conditions, we present results from a suite of failure experiments on basalt under general stress states. Compression and tension/torsion Kolsky bars are used to illustrate the dynamic (100-1000 1/s) compressive, tensile, and shear responses of the material. Quasi-static compression experiments are used to determine deformation mechanisms at low rates (10^{-1}-10^{-4} 1/s). Using results from these experiments, the evolution of strength and damage mechanisms with strain rate can be examined. High-speed imaging (frames every 2-4 \(\mu\)sec) is used to illustrate crack speeds and failure processes during experiments, while post-mortem SEM analysis provides information about fracture surfaces and relevant damage mechanisms across strain rates.

5:15PM L5.00007 Anisotropic elastic-plastic transition of MgO under shock compression , XUN LIU, KENICHI OGATA, Shock Wave and Condensed Matter Research Center, Kumamoto University, XIANMING ZHOU, National Key Laboratory of shock Wave and Detonation Physics, Institute of Fluid Physics, WILLIAMS J. NELLIS, Department of Physics, Harvard University, TOSHIMORI SEKINE, Department of Earth and Planetary Systems Science, Hiroshima University, TSUMOTO MASHIMO, Shock Wave and Condensed Matter Research Center, Kumamoto University — The failure of brittle materials under uniaxial shock-loading has been the subject of many discussions. But the physical explanation of the yield behavior remains poorly understood. In this study, we focus on the elastic-plastic transition of MgO single crystal, which is the simplest metal oxide with a cubic structure, and can be studied as a prototype. Otherwise, the equation of state (EOS) of MgO is also a key problem because of its geophysical importance and its application as pressure scale in static compression experiments. The interface particle velocity profile between MgO single crystal and LiF window was measured by a VISAR system. The Hugoniot elastic limits (HELs) along <100> direction are measured to be around 4.2 GPa, and keep constant under different loading pressure, while the HELs along <110> direction is much higher, with a minimum value of 10GPa and increase with final pressure. When shock along <100> direction, MgO suffers a catastrophically loss of shear strength, while along <110> direction, the deformation is more close to ideal elastic-plastic change. These differences indicate different deformation mechanism along different loading direction, which will be discussed later.

Tuesday, July 9, 2013 3:30PM - 5:30PM –
Session L6 CH.2 Chemistry: Metal Hydrides and Nitrides Cascade II - Ranga Dias, Washington State University

3:30PM L6.00001 Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides\(^1\) , EVA ZUREK, University at Buffalo, SUNY — Stabilization of solid phases with unusual combinations or stoichiometries, and unexpected electronic structures may be achieved by applying external pressure. The prediction of these structures using our chemical intuition (developed at 1 atmosphere) would be exceedingly difficult, making automated structure search techniques prudent. For this reason, we have written XtalOpt, an open-source evolutionary algorithm for crystal structure prediction. Whereas at 1 atmosphere the classic alkali hydrides combine in a one-to-one ratio, M\(^+\)\(+\), under pressure non-classic stoichiometries MH\(_n\)(\(n > 1\)) and M\(_n\)H\(_{m}\)(\(m > 1\)) are preferred. For example, theoretical work has predicted that LiH\(_n\) and NaH\(_n\) become particularly stable phases at about 100 and 25 GPa, respectively. And the potassium, rubidium and cesium polyhydrides all contain the H\(_3\)\(^-\) anion, the simplest exape of a three centered four electron bond. The alkaline-earth polyhydrides are considered as well. Chemical trends relating the stabilization pressure to the ionization potential, and the nature of the hydrogenic sublattice to the strength of the metal-hydride interaction can be made. These hydrogen-rich materials with nontraditional stoichiometries are computed to undergo an insulator to metal transition at pressures attainable in diamond anvil cells. It may be that these systems are superconductors at experimentally achievable pressures. The metal-rich region of the alkali/hydrogen phase diagram under pressure shows that alkali-metal subhydrides may also be stabilized under pressure.

\(^1\)We acknowledge the NSF (DMR-1005413) for financial support.
4:00PM L6.00002 Phase Transition of Rare-earth Metal Hydrides under High Pressure

YOUNG KIM, Geophysical Laboratory, Carnegie Institution of Washington D.C. — Hydrogen is the lightest and smallest element in the periodic table. Despite its most simple electronic structure, enormous complexity can arise when hydrogen participates in the formation of solids. High pressure perturbs the free energy sufficiently to push the system into unexplored regions of the energy landscape, thus providing an excellent platform for the investigation of novel physics in hydrides such as metal-insulator transition, superconductivity as well as stoichiometric change. In this talk, I will overview recent progress on hydrides research under pressure in both theoretical works and experiments. Theoretical predictions on atomic positions and stoichiometry in hydrides under high pressure play a critical role to determine crystal structures of experimentally observed novel compounds, especially due to tiny scattering length of hydrogen atoms in solids. In addition, predicted physical property such as metallization and superconductivity in hydrides can guide experiments and experimental observations provide inputs for refinement of calculations I will show examples to highlight the importance of integrated experiment-theory collaboration to study rare-earth hydride under high-pressure.

1Energy Frontier Research in Extreme Environments (EFREE) Center

4:30PM L6.00003 High-density Modifications in Hydrogen-Rich Compound Diborane

SERGE DESGRENIERS, Physics, U. of Ottawa, Canada, AKIO YOSHINAKA, Physics, U. of Ottawa, Canada, YANSUN YAO, Physics and Engineering Physics, U. of Saskatchewan, Canada, DENNIS KLUG, National Research Council of Canada — The study of dense hydrogen-rich compounds is regarded as a way to investigate pathways to metallic hydrogen. Compression of hydrides may lead to a metallic state at lower pressures than that required for hydrogen. Condensed diborane represents an interesting hydride as its high dipole polarizability yields to a prediction of a metallic state below 100 GPa. And, at lower density, theoretical results indicate the possible formation of complex molecular crystal structures, as a function of compression, comprising not only dimers of B_{2}H_{4} but also higher order molecular assemblies, (BH_{n})_{2}, with n > 2, and even polymeric chains. In this contribution, experimental results characterizing condensed phases of diborane, as obtained at high pressure at room temperature, are compared to predicted crystalline structures. Raman spectroscopy and x-ray diffraction with synchrotron radiation were carried out on single crystal as well as polycrystalline samples in diamond anvil cells for pressures up to 85 GPa. Results obtained at low pressures (<4 GPa), across the liquid-solid phase boundary, indicate the existence of a phase with a crystalline structure different from that of the known b-phase (P2_{1}/n). Solid-to-solid transitions are observed at 6 and 14 GPa. The crystalline structures of the high-pressure phases, obtained by X-ray diffraction, are compared to molecular assemblies obtained theoretically. Finally, the possible metallization at high pressure is explored.

4:45PM L6.00004 Disproportionation reaction of LaH_{2} at high pressure and low temperature

AKIHIKO MACHIDA, TETSU WATANUKI, DAICHI KAWANA. KATSUTOSHI AOKI, Quantum Beam Science Directorate, Japan Atomic Energy Agency, Japan — We have found that fcc-LaH_{2} decomposes into two phases, which have different hydrogen compositions, a H-poor and H-rich phases, at 11 GPa at room temperature through synchrotron radiation x-ray diffraction (SR-XRD) measurements. The decomposition proceeds spontaneously by pressurization, being interpreted in terms of a disproportionation reaction. Recent neutron diffraction measurements on LaD_{2} confirmed the formation of a NaCl-type LaD as the D-poor phase. The disproportionation accompanies the transfer of H atoms from the tetrahedral to octahedral interstitial sites in the fcc metal lattice. The diffusivity of the H atoms in the metal lattice would be suppressed at low temperature. We hence investigated the pressure-induced disproportionation at low temperature by SR-XRD measurements at BL22XU, SPring-8, and found the disproportionation occurred at 13.5 GPa even at 200 K. The volume fraction of the H-poor phase relative to the H-rich one at 200 K was larger than that of the H-poor phase at room temperature. The H-transfer by the disproportionation will be discussed in terms of temperature effect.

5:00PM L6.00005 New routes to nitrogen-rich transition metal nitrides: Synthesis of novel polymorphs of Hf_{3}N_{2}

ASHKAN SALAMAT, Harvard University, A.L. HECTOR, B.M. GRAY, Southampton University, S.A. J. KIMBER, European Synchrotron Radiation Facility, P. BOUVIER, CNRS, P.F. MCMILLAN, University College London — One of the most obvious features of transition metal nitride chemistry is that the maximum formal oxidation state of the metal is rarely as high as in the corresponding oxides or fluorides. Much of the interest in the high oxidation phases has come from the desire to identify the next generation of photocatalytic materials with tuneable bandgaps. Experiments in the laser heated diamond anvil cell (LHDAC) between the direct reaction of metals and nitrogen have previously produced a number of important new main group nitride phases. This technique has also demonstrated its potential for formation of new nitrogen-rich transition metal nitride phases. Alternative methods with the development of “soft” routes to new phases with high nitrogen content also offer the possibility of obtaining metastable phases through topotactic conversions. Using LHDAC in situ with synchrotron angle dispersive diffraction techniques we have crystallised at high pressures and temperatures two novel polymorphs of Hf_{3}N_{2}. Starting with an amide-derived nanocrystalline Hf_{3}N_{2} sample we have identified a novel tetragonal (I4/m) polymorph at 15 GPa and 1500 K and a second high pressure orthorhombic (Pnma) polymorph at 30 GPa and 2000 K. This study demonstrates that the combination of precursor-based synthesis and high-pressure crystallization could be very productive in synthesis of such nitrogen-rich phases.

5:15PM L6.00006 Physical and chemical transformations of iron pentacarbonyl under pressure

YOUNG YAY RYU, Institution for Shock Physics, Department of Material Science and Engineering and Department of Chemistry Washington State University, CHOONG SHIH YOO, Washington State University — We have studied the physical and chemical transformations of iron pentacarbonyl (Fe(CO)_{5}) in externally-heated diamond anvil cells using in situ micro-Raman and synchrotron x-ray diffraction. Raman spectra of Fe(CO)_{5} are most characteristic to three different solid polymers and a polymeric solid found at high pressure-temperature condition, yielding the phase/chemical transformation diagram to 650 K and 20 GPa. The spectral results, for example, reveal that liquid Fe(CO)_{5} undergoes several phase transformations to metastable solid phase I at 0.3 GPa, phase II at 1.5 GPa, and phase III at 4.8 GPa that polymerizes above 16 GPa. The X-ray diffraction data support the phase transitions that were observed in the Raman spectroscopy. These polymers also exhibit distinctive crystal morphology and optical properties, which will be discussed in this paper.

1The work has been performed in support of the DTRA (Grant No. HDTRA-12-1-0020).

Tuesday, July 9, 2013 3:30PM - 5:15PM –
Session L7 CM.1 Equation of State: Fluids — Grand Crescent - Gabriel Gwanmesi, Delaware State University
3:30PM L7.00001 Experimental Measurement of Speeds of Sound in Liquid Carbon Monoxide and Development of High-Pressure, High-Temperature Equations of State. JOSEPH ZAUG, Lawrence Livermore National Laboratory, JEFFREY CARTER, Picarro.com, SORIN BASTEA, MICHAEL ARMSTRONG, FRIED LAURENCE, Lawrence Livermore National Laboratory — We report the adiabatic sound speeds for supercritical fluid carbon monoxide along two isotherms, from 0.17 to 2.13 GPa at 297 K and from 0.31 to 3.2 GPa at 600 K. The carbon monoxide was confined in a resistively heated diamond-anvil cell and the sound speed measurements were conducted in situ using a recently reported variant of the photoacoustic light scattering effect. The measured sound speeds were then used to parameterize a single site dipolar exponential-6 intermolecular potential for carbon monoxide. PT thermodynamic states, sound speeds, and shock Hugoniot results were calculated using the newly parameterized intermolecular potential and compared to previously reported experimental results. Additionally, we generated an analytical equation of state for carbon monoxide by fitting to a grid of calculated PT states over a range of 0.1-10 GPa and 150-2000 K. A 2 percent mean variation was found between computed high-pressure solid-phase densities and measured data - a surprising result for a spherical interaction potential. We further computed a rotationally dependent fluid to beta-phase boundary; results signal the relative magnitude of short-range rotational disorder under conditions that span existing boundary measurements.

3:45PM L7.00002 Shock Compression of Cryogenic Noble Gas Mixtures: Xenon – Krypton. SETH ROOT, RUDOLPH MAGARY, RAYMOND LEMKE, THOMAS MATTSSON, Sandia National Laboratories — In past work, we have examined the multi-Mbar response of cryogenically cooled liquid xenon and liquid krypton measuring their Hugoniots to 8 Mbar. These results were utilized in the development of new EOS models for Xe and Kr to use in high energy density physics applications. The previous work demonstrated the usefulness of integrating high accuracy shock compression experiments with DFT to generate the basis for equation of state (EOS) models. In many physics applications, such as Z-pinch experiments, gas mixtures are used instead. However, we do not have reliable experimental data on these mixtures to provide informed decisions about the EOS models or mixture rules. To improve our understanding of mixtures at extreme conditions, we performed dynamic compression experiments using Sandia’s Z – facility on a 70/30 molar ratio Kr/Xe cryogenically cooled liquid mixture. We measured the Hugoniot state and reshock state of the liquid mixture to several Mbar. The experimental data validated the DFT simulations for identical molar ratio mixtures. The combined experimental and DFT results are used to assess the EOS models and test the mixture rules. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

4:00PM L7.00003 Temperature Measurements in Shocked Liquid Benzene and an Improved Benzene EOS. DAVID LACINA, Y.M. GUPTA, Washington State University — Time-resolved Raman spectroscopy measurements were used to determine temperatures in multiply-shocked liquid benzene to peak pressures of ~19GPa. Experimentally determined temperatures were obtained using the ratio of anti-Stokes to Stokes scattering intensities for the 992cm⁻¹ vibrational mode. Our experimental results demonstrate that the calculated temperatures obtained using the current benzene equation of state (EOS) [S. Root, Ph.D. Thesis, WSU], though reasonable, are consistently lower than the measurements. To improve calculated temperatures, key thermodynamic parameters (e.g. the specific heat) in the current benzene EOS were varied to examine and understand the sensitivity of temperatures to those parameters. Specific heat variations, as expected, resulted in the largest change in the calculated parameters. Building on the sensitivity studies, the benzene EOS was refined to produce a good agreement between the calculated temperatures and the measured temperatures in multi-paddle shocked benzene. The improved EOS resulted in a higher decomposition temperature for singly shocked liquid benzene.

4:15PM L7.00004 Shock Hugoniot Equations of State for BinaryIdeal (Toluene/Fluorobenzene) and Non-Ideal (Ethanol/water) Liquid Mixtures. PETER SCHULZE, NHAN DANG, CYNTHIA BOLME, KATHRYN BROWN, SHAWN MCGRANE, DAVID MOORE, Los Alamos National Laboratory, HERCULES TEAM — Laser shock Hugoniot data were obtained using ultrafast dynamic ellipsometry (UDE) for both non-ideal (ethanol/water solutions with mole percent $x_{\text{ethanol}} = 0, 3.4\%, 7.5\%, 11\%, 18\%, 33\%, 56\%, 100\%$) and ideal liquid mixtures (toluene/fluorobenzene solutions with mole percent $x_{\text{toluene}} = 0\%, 26.0\%, 49.1\%, 74.9\%, 100\%$). The shock and particle velocities obtained from the UDE data were compared to the universal liquid Hugoniot (ULH) equation. It was found that the UDE data deviate below the ULH for water and trend upward with respect to the ULH with increasing ethanol fraction, finally deviating completely above the ULH for mixtures with mole fraction greater than or equal to 56%. However, the ethanol/water mixture UDE data do not monotonically transition from below the ULH to above the ULH across the concentration range, but instead show increased deviation between ethanol mole fraction 7% - 12%. In contrast, the UDE data from the ideal liquid mixture are well behaved and agree with the ULH prediction across the concentration range. The deviations of the non-ideal ethanol/water data from the ULH are attributed to complex hydrogen bonding networks in ethanol/water mixtures that alter the compressibility of the mixture.

4:30PM L7.00005 The Equation of State of Water in the MPa to TPa Regime. J. MICHAEL BROWN, Earth and Space Sciences, University of Washington — The thermodynamic properties of water, in continual refinement on the basis of evolving experimental and theoretical methods, span an enormous range of volume, temperature, and pressure. A current generation equation of state can accurately represent experimental data below 100 MPa but fails to match with experimental uncertainties a body of high-pressure data. B-spline basis functions (piece-wise continuous polynomials) lend themselves to regularized linear and non-linear inverse techniques and can represent equation of state surfaces. Here, a sixth order tensor b-spline for the free energy is used to fit sound speeds, specific heats, densities, and thermal expansivities in accord with estimated uncertainties. This framework for the assimilation of data allows for flexible fitting to arbitrary precision. Once a system is adequately represented, revisions are easily accomplished in the face of new data or revised interpretations. The new equation of state fits low-pressure data as well as static and shock data extending to more than 100 GPa. Since this representation contains no theoretical assumptions, it provides an unbiased estimator for comparisons with theory. For example, super ionic behavior in the fluid phase is evaluated.

4:45PM L7.00006 Warm dense water in 100 GPa regime. NORIMASA OZAKI, Osaka University, TOMOAKI KIMURA, Ehime University, TAKUO OKUCHI, Okayama University, MARTIN FRENCHE, University of Rostock, TOMOYUKI KAKESHIYA, MIKA KITA, KOHEI MIYANISHI, Osaka University, RONALD REDMER, University of Rostock, TAKAYOSHI SANO, TOMOKAZU SANO, KATSUYA SHIMIZU, TOMOYUKI TERAI, Osaka University, RYOSUKE KODAMA, Graduate School of Engineering, Osaka University — We have experimentally measured the pressure-volume-temperature equation-of-state and the optical reflectivity of water, which matches with the interior condition of the water-rich super Earth. Transition between the warm dense fluid water and the electronically conducting fluid, where its physical and chemical properties are changing dramatically (~100 GPa range) has been explored with experiments that can directly measure the temperature of the system. It can be done by focusing strong laser onto a preloaded water. Understanding of the inner structure of such unique super-Earths would be a key constraint on the origin and evolution of exoplanetary systems.
5:00PM L7.00007 Thermodynamics of Dynamically Compressed Gases at Megabar Pressures
VICTOR GRYAZNOV, Institute of Problems of Chemical Physics RAS, IGOR IOSILEVSKII, Joint Institute for High Temperatures RAS, EUGENE YAKUB, Cybernetics Department, Odessa National Economic University, VLADIMIR FORTOV, Joint Institute for High Temperatures RAS — Thermodynamic model based on "chemical picture" is applied to calculation of equation of state of warm dense hydrogen, deuterium and helium at submegabar and megabar pressure range. Strongly compressed fluid is considered as a multi-component strongly interacted mixture of atoms, molecules, ions and electrons. Nonideality effects of Coulomb interaction of charged particles and short-range repulsion of atoms and molecules are included in thermodynamic functions as well as in effective shifts of ionization and dissociation equilibrium. Effects of free electrons degeneracy are taken into account in charge screening. The results of calculation of principal Hugoniots of hydrogen and deuterium at submegabar pressures are compared with experimental data and calculations by means of ab initio DFT-MD approach and calculations on the basis of non-empirical atom-atomic approximation. New calculations of Hugoniots of high density precompressed deuterium at megabar pressures and extended density range are presented. The results of calculations of thermodynamic functions for isentropic compression of helium at multi-megabar pressures are presented and compared with experimental data and DFT-MD data. Contribution of various plasma effects, such as dissociation of molecular phase, ionization, interparticle interaction, degeneracy effects of free electrons whole range of pressures covered by the experiments are analyzed and discussed.

5:30PM - 5:30PM Session M1 Poster Session II (5:30 - 7:00PM) Grand Ballroom I -

M1.00001 Laser drive development for the APS Dynamic Compression Sector
THOMAS LAGRANGE, DAMIAN SWIFT, BRYAN REED, JOEL BERNIER, MUKUL KUMAR, JAMES HAWRELIAK, JON EGGERT, SHAM DIXIT, GILBERT COLLINS, Lawrence Livermore National Laboratory — The Dynamic Compression Sector (DCS) at the APS synchrotron offers unprecedented possibilities for x-ray diffraction and scattering measurements in-situ during dynamic loading, including single-shot data collection with x-ray energies high enough (tens of keV) to study high-Z samples in transmission as well as reflection. Dynamic loading induced by laser ablation is an important component of load generation, as the duration, strain rate, and pressure can be controlled via the energy, spot size, and pulse shape. Using radiation hydrodynamics simulations, validated by experiments at several laser facilities, we have investigated the relationship between irradiance history and pressure for ablative loads designed to induce shock and ramp loading in the nanosecond to microsecond range, and including free ablation and also ablation confined by a transparent substrate. We have investigated the effects of lateral release, which constrains the minimum diameter of the focal spot for a given drive duration. In this way, we are able to relate the desired drive conditions to the total laser energy needed, which dictates the laser technologies suitable for a given type of experiment.

M1.00002 X-ray Thomson scattering as a temperature probe for gigabar shock experiments
T. DOEPPNER, A. KRITCHER, S. GLENZER, Lawrence Livermore National Laboratory, D. CHAPMAN, AWE Aldermaston, R. FALCONE, University of California - Berkeley, P. NEUMAYER, GSI Darmstadt — In X-ray Thomson scattering (XRTS), high-resolution spectrometry of probe x-rays scattered from matter gives an elastic (ionic) and an inelastic (electronic) feature, whose location, width, and amplitude can be analyzed for the temperature and density of the electrons. This diagnosis is complementary to traditional, mechanical EOS measurements which do not directly constrain temperature. XRTS has been demonstrated on planar dynamic-loading experiments at the Omega laser, and a spectrometer has been constructed for use at the National Ignition Facility (NIF). We plan to obtain XRTS measurements into the gigabar regime using hohlraum-driven converging shocks at NIF. In these experiments, the radial profile through the sample at any instant of time varies greatly, though the XRTS signal is dominated by the hottest region, which is at the shock front where simultaneous radiography obtains an equation of state measurement. However, the shock signal is potentially obscured by scattering from the preheat shield, comprising a higher-Z dopant than the sample. Thus we are developing an imaging spectrometer, which should enable a spatial unfold of XRTS spectrum, providing a more precise temperature measurement at the shock front and potentially in the converging flow behind the shock.

M1.00003 Synchronizing flash-melting in a diamond cell with synchrotron X ray diffraction (XRD)
AMOL KARANDIKAR, REINHARD BOEHLER, Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road NW, Washington, DC 20015, USA, YUE MENG, ERIC ROD, GUOYIN SHEN, HPCAT, Geophysical Laboratory, Carnegie Institution of Washington, Arcoone, Illinois 60439, USA — The major challenges in measuring melting temperatures in laser heated diamond cells are sample instability, thermal runaway and chemical reactions. To circumvent these problems, we developed a "flash heating" method using a modulated CW fiber laser and fast X-ray detection capability at APS (Pilatus 1M detector). As an example, Pt spheres of 5micron diameter were loaded in a single crystal sapphire encapsulation in the diamond cell at 65 GPa and heated in a single flash heating event for 20ms to reach a desired temperature. A CCD spectrometer and the Pilatus were synchronized to measure the temperature and the XRD signal, respectively, when the sample reached the thermal steady state. Each successive flash heating was done at a higher temperature. The integrated XRD pattern, collected during and after (300K) each heating, showed no chemical reaction up to 3639K, the highest temperature reached in the experiment. Pt111 and 200 peak intensity variation showed gradual recrystalization and complete diminishing at about 3660 K, indicating melting. Thus, synchronized flash heating with novel sample encapsulation circumvents previous notorious problems and enables accurate melting temperature measurement in the diamond cell using synchrotron XRD probe.

M1.00004 New pressure cell for ultrasonic measurements
MICHAL KEGA, ANDREW HUXLEY, KONSTANTIN KAMENEV, University of Edinburgh — Ultrasonic interferometry at high pressure remains a technical challenge as the small sample space requires the application of very high-frequency ultrasound [1]. Here we present the design of a new cell developed specifically for ultrasonic measurements of single crystals at low temperatures (2K) and high pressures (5GPa). The design allows greater sample space (compared to a conventional diamond anvil cell) and simultaneous measurement of ultrasonic attenuation and velocities. Coupling the fine transducers to spherical sapphire anvils reduces background and enables different polycrystalline samples to be measured at the same pressure and temperature conditions. The results are used to deduce the elastic, electronic and magnetic properties of a crystal. The finite element analysis of the cell together with the pressure calibration curves and test data taken on UGe2 are presented.

J.-P. Davis, J. Appl. Phys. 99, high brilliance and coherence of the FEL radiation will enable spatially resolved studies. Spectroscopy. The high intensity and time structure will enable time-resolved studies of the samples generated during dynamic compression. In addition, the high excitation energies, diffraction patterns will have excellent quality and a wide range of elements ($Z > 22$) will be accessible at hard X-ray sources up to 10 Mbar at comparatively low temperatures. A suitable optical laser system with repetition rates of 0.1 and 10 Hz was developed to be used in the Paris-Edinburgh Cell.

— The European XFEL [1] plans to integrate a nanosecond pulse duration laser system into the high energy density experiment (HED) to enable studies of non-uniform materials under pressure. The Paris-Edinburgh press enables us to compress large volume samples up to 2 mm in both diameter and length up to ~ 7 GPa and 2300 K. The resolution of white x-ray radiography is ~ 4 μm. The ultrasonic wave velocity measurement can be made for liquid materials as well as amorphous solids. The falling sphere viscometry technique have been developed using high-speed x-ray camera (>1000 frame/second), enabling us to investigate viscosity of not only high viscosity melts such as silicates but also low viscosity (<1 mPa s) liquids such as liquid metals and salts.

M1.00005 Integration of structure, x-ray radiography, elastic wave velocity, and viscosity measurement in the Paris-Edinburgh Cell. YOSHIO KONO, CHANGYONG PARK, CURTIS KENNEY-BENSON, GUOYIN SHEN, HPCAT, Geophysical Laboratory, Carnegie Institution of Washington, YANBIN WANG, GSECARS, the University of Chicago — We have integrated a range of techniques for physical property measurement with the energy-dispersive x-ray diffraction (EDXD) technique at the 16BM-B, a white x-ray beamline at the Advanced Photon Source, to promote comprehensive studies of structure-property correlations of liquid and amorphous materials at high-pressure. These include white x-ray radiography, ultrasonic velocity, and falling sphere viscometry techniques. The integration is centered on a Paris-Edinburgh cell to fully utilize the multi-angle EDXD capability with the wide open access. The integrated techniques are particularly useful to study liquid and amorphous materials, for which the integrated facility allows making simultaneous observations over a range of pressures and temperatures from the direct manifestation of the microscopic structure, to the high excitation energies, diffraction patterns will have excellent quality and a wide range of elements ($Z > 22$) will be accessible at hard X-ray sources up to 10 Mbar at comparatively low temperatures. A suitable optical laser system with repetition rates of 0.1 and 10 Hz was developed to be used in the Paris-Edinburgh Cell.

M1.00006 Development of multi-component explosive lenses for arbitrary phase velocity generation. JASON LOISEAU, JUSTIN HUNEALI, OREN PETEL, SAM GOROSHIN, DAVID FROST, ANDREW HIGGINS, McGill University, Mechanical Engineering Dept., 817 Sherbrooke St. W., Montreal, Quebec, H3A 2K6, Canada, FAN ZHANG, Defence R&D Canada - Suffield, PO Box 4000, Station Main, Medicine Hat, Alberta, T1A BK6, Canada — The combination of explosives with different detonation velocities and lens-like geometric shaping is a well-established technique for producing structured detonation waves. This technique can be extended to produce nearly arbitrary detonation phase velocities for the purposes of sequentially imploding pressurized tubes or driving Mach disks through high-density metalized explosives. The current study presents the experimental development of acceleration, multi-component lenses designed using simple geometric optics and idealized front curvature. The fast explosive component is either Composition C4 (VOD = 8 km/s) or Primasheet 1000 (VOD = 7 km/s), while the slow component varies from heavily amine-diluted nitromethane (amine mass fraction exceeding 20%) to packed metal and glass particle beds wetted with amine-sensitized nitromethane. The applicability of the geometric optic analog to such highly heterogeneous explosives is also investigated. The multi-layered lens technique is further developed as a means of generating a directed mass and momentum flux of metal particles via Mach-disk formation and jetting in circular and oval planar lenses.

M1.00007 Investigation of non-uniform materials under pressure. VLADIMIR SICHENNIKOV, IGOR KORBEYNIKOV, NATALIA MOROZOVA, VSEVOLOD SICHENNIKOV JR., VLADIMIR VORONIN, IVAN BERGER, Institute of Metal Physics of RAS, Urals Division, Yekaterinburg, 620990, Russia, LABORATORY OF ELECTRONIC PROPERTIES OF MATTER AT HIGH PRESSURES TEAM, LABORATORY OF NEUTRON INVESTIGATION OF MATTER TEAM, LABORATORY OF MICROMECHANICS TEAM — The approach is considered of the investigation of non-uniform (NU) materials at high pressure (P). Under P a material may become NU due to phase transition (PT). At topological insulators the properties may include the contributions both of the bulk states as well as of the surface ones as at NU material etc. The approach is based on the model of multi-phase system with ordered phase inclusions of variable configuration (A) and concentration (C), and the experimental data are presented for: i) the substances near PT, ii) some ceramics, iii) the certain natural minerals. Si, ZnX, PbX, SmX (X = Te, Se, S), GaP, iron ores, and (WC)$_n$(Co)$_{1-x}$ hard alloys etc. have been investigated under P up to 30 GPa. It was shown that the model allows to describe resistance (R) and thermoelectric power (S), etc. in the vicinity of PT. For hard alloys WC-Co the elastic modulus has been fitted using the model, and A has been estimated to be distinguished from the simple isotropic case. In the iron ores the A and the C of various components (Fe, Fe$_3$O$_4$, MgO, Mg$_2$SiO$_4$, etc.) has been estimated due to the using of the new approach based on the different depth of penetration of X-ray and neutron radiation, and also on different dependences of S, R on C, A.

M1.00008 Dynamics of shocks in laser-launched flyer plates probed by photon Doppler velocimetry. ALEXANDER CURTIS, DANA DLOTT, UIUC — We have developed a laser-launched flyer plate system that lets us launch Al flyers of varying thicknesses at velocities up to 4 km/s using different duration laser pulses. We probe the launch and impact with a target using an 8 GHz PDV system. These 25-100 micron thick flyers produce shocks lasting a few nanoseconds. The launch process involves generating a shock in the Al foil that rings and damps out. When the flyer impacts a target, a complicated shock waveform is generated including a steady shock and a release wave. The duration of the steady shock, usually thought to be about equal to the shock round-trip time in the flyer plate, turns out to be quite different. These phenomena were studied in detail using PDV, and their dynamics depend a great deal on the launch laser pulse duration and the flyer thickness. Of particular interest is how the viscoelastic relaxation of the polymer PMMA depends on shock duration in the short shock regime.

M1.00009 Raman Temperature Measurement. DAVID MOORE, SHAWN MCGCRANE, Los Alamos National Lab — We are examining the experimental tradeoffs for the use of the spontaneous Raman Stokes/anti-Stokes intensity ratio as a fundamental temperature measurement at static and dynamic extreme conditions. The tradeoff space includes spatial resolution and temperature range versus vibrational frequency, as well as heating of the sample and nonlinear damage caused by the excitation laser. The experiments are being performed under a range of experimental conditions from picoseconds to seconds and from cryogenic (77 K) to elevated (ca. 1000 K) temperatures. The results are being compared to calculations for transparent metal oxide, polymer, and inorganic materials, with the aim to demonstrate their potential as temperature reporters when used as thin windows on opaque materials.

M1.00010 Extreme pressure research at the European XFEL. KAREN APPEL, European XFEL, THOMAS COWAN, Helmholtz-Zentrum Dresden Rossendorf, HANNS-PETER LIERMANN, DESY, MOTOAKI NAKATSUSUMI, THOMAS TSCHENTSCHER, European XFEL. The European XFEL [1] plans to integrate a nanosecond pulse duration laser system into the high energy density experiment (HED) to enable studies of materials at extremely high pressures. Ramp-compression [2] by nanosecond shaped laser pulses will enable to extend the range of high pressure conditions accessible at hard X-ray sources up to 10 Mbar at comparatively low temperatures. A suitable optical laser system with repetition rates of 0.1 and 10 Hz was recently proposed by an international consortium. Probing of the laser generated excited states will be performed with the high energy X-ray free electron laser (FEL). In the energy range between 5 and 25 keV, it will be possible to study samples by X-ray diffraction, X-ray spectroscopy and imaging techniques. Due to the high excitation energies, diffraction patterns will have excellent quality and a wide range of elements ($Z > 22$) will be accessible by X-ray absorption spectroscopy. The high intensity and time structure will enable time-resolved studies of the samples generated during dynamic compression. In addition, the high brilliance and coherence of the FEL radiation will enable spatially resolved studies.

[1] for detailed information about European XFEL see www.xfel.eu
M1.00011 Extraction of the pressure dependence of the bulk sound velocity of metals from the calculated precompressed Hugoniot in laser-driven shock wave experiments, NOA NISSIM, SHALOM ELIEZER, MEIR WERDIGER, LIOR PERELMUTTER, Sorok NRC, APPLIED PHYSICS DEPARTMENT TEAM — Recently [1] a novel route to approach the cold compression curve in laser-plasma induced shock waves was suggested. This effect is achieved with a precompression in a diamond anvil cell (DAC). In order to keep the necessary structure of one dimensional shock wave it is required to use a diamond anvil cell with a partially perforated diamond anvil. Precompression pressures of about 50 GPa, that are of an order of magnitude higher than the currently reported pressures, are possible to obtain with presently existing diamond anvil cell technology. In this paper, precompressed Hugoniot curves for Al, W and Ta were calculated up to 15 Mbar for different initial pressures reaching to 50 GPa. From the calculated precompressed Hugoniot curves of Al, W and Ta the pressure dependence of the bulk sound velocity was extracted and was used as a consistency check for the calculations’ assumptions. It was found that this method provides a good prediction to the pressure dependence of the bulk sound velocity of metals.


M1.00012 Characterization of epoxy-based encapsulents, JAMES WILGEROTH, ANNA KHAN, JENS BALZER, Imperial College London, INSTITUTE OF SHOCK PHYSICS TEAM — A range of experiments have been performed in order to investigate the effects of strain-rate on the compressive response of both an epoxy resin and an epoxy-based syntactic foam. Strain-rates ranging from the quasi-static (10^{-4} s^{-1}) to dynamic (10^{3} s^{-1}) regime have been investigated using an Instron 5584 Universal Testing Machine and Split-Hopkinson Pressure Bar (SHPB) apparatus. The effects of temperature (-20 to 80°C) on the compressive response of the materials have also been investigated. Finally, the experimental results are discussed with reference to the wider challenge of numerical simulation.

M1.00013 Models of the Dynamic Deformations of Polymers, LEV MERZHIEVSKY, professor, MIHAIL VORONIN, ANNA KORCHAGINA, None — In the process of deformation under the influence of external loading polymeric mediums show the complicated behavior connected with features of their structure. For amorphous polymers distinguish three physical conditions — glasslike, highelastic and viscoplastic. To each of the listed conditions there corresponds to micro - meso- and macrostructural mechanisms of irreversible deformation. In the report the review of results of construction of models for the description of dynamic and shock-wave deformation of the polymers which are based on developed authors representations about mechanisms of irreversible deformation is made. Models include the formulation of the equations of conservation laws, considering effect of a relaxation of shear stresses in the process of deformation. For closing of models the equations of states with nonspherical tensor of deformations and relation for time of a relaxation of shear stresses are constructed. With using of the formulated models a number of problems of dynamic and shock wave deformations has been solved. The results are compared with corresponding experimental date. Development of the used approach are in summary discussed. To taking into account memory and fractal properties of real polymers it is supposed of derivatives and integrals of a fractional order to use. Examples of constitutive equations with derivatives of a fractional order are presented. This work is supported by the Integration project of the Siberian Branch of the Russian Academy of Science 64 and grant RFBR 12-01-00726.

M1.00014 Heterogeneous deformation of metals (copper, tantalum, uranium, titanium) at convergence of cylindrical apertures having small diameters under effect of shock waves, MALY-SHEV ANDREY, ZAMOTAEV DMITRIY, IGNATOVA OLGA, TKACHENKO MICHAL, SHEPELEV ERICH, TYUPANOVA OLGA, PODURETS ALEKSEY, Balandina Anna, Kondrokhina irina, None — Construction metals undergo loadings of various types during high-velocity deformation. As a result, there are different structural changes and, in particular, varying of mechanical properties. One of these complex structural changes is the process of formation of heterogeneous localized shear bands (LSB) of the twinning nature and the associated temporal decrease of dynamic strength in strong shock waves. The earlier investigations in this area point to the fact that the process of LSB formation has the threshold character, and pressure is the main criterion. So, it is shown in work that LSB formation occurs in coarse-grained copper after effect of shock wave with the amplitude 28-30 GPa. In this work, within the investigation of convergence of cylindrical channels having small diameters under effect of planar shock waves, it is shown that LSB can be formed in metals, and flow stops being homogeneous at rather low loading level (up to 10 GPa). In this case, the level of plastic strain and its rate are the main factors, which are responsible for heterogeneous deformation. The authors present results of experimental and metallographic researches for some metals, which are copper with various grain sizes, tantalum, uranium, and titanium alloys.

M1.00015 Laser-driven focusing surface shock waves in glass, DAVID VEYSSET, ALEX MAZNEV, MIT, THOMAS PEZERIL, Université du Maine, STEVE KOOI, KEITH A. NELSON, MIT — Direct real-time visualization of converging surface shock waves in glass is demonstrated in an all-optical experiment. The optical set-up includes an axicon that focuses an intense picosecond excitation pulse into a ring-shaped pattern at the surface of a gold coated glass substrate. Optical excitation induces surface acoustic waves that propagate in the plane of the sample and converges toward the center resulting in cylindrical focusing of the shock front. The nonlinear evolution of the SAWs and the shock formation is observed at the micro-scale using interferometry with a femtosecond probe pulse at variable delays. A series of images is obtained tracing the converging wave as it collapses in the focal point. The quantitative analysis of the full-field images provides direct information about the surface displacement and the shock velocity. The results open the prospect of spatially resolved studies of shock-compressed materials in a small-scale all-optical experiment.

M1.00016 Origin of the Volume Collapse under Pressure in Elemental Pr and Gd, JINHYUK LIM, Washington University in St. Louis, TAKAHIRO MATSUOKA, Osaka University, GILBERTO FABBRI, Argonne National Laboratory/Washington University in St. Louis, KATSUYA SHIMIZU, Osaka University, DANIEL HASKEL, Argonne National Laboratory, JAMES SCHILLING, Washington University in St. Louis — Most lanthanide metals exhibit a volume collapse at a critical pressure P_c. The primary mechanism responsible for this collapse is a matter of debate and may involve the 4f electrons themselves or be the result of simple s − d transfer in the conduction electrons. Possible pressure-induced changes in the 4f electron system include: (i) valence increase, (ii) 4f/4band formation, and (iii) increased 4f-conduction electron hybridization leading to Kondo volume collapse. The results of published synchrotron spectroscopic studies at pressures near P_c (21 GPa for Pr and 59 GPa for Gd) will be critically examined. Recent high-pressure experiments on the dilute magnetic alloys Y(Pr) and Y(Gd) shed light on the appropriateness of the Kondo volume collapse model for elemental Pr and Gd. In Y(Pr) or Y(Gd) the superconductivity of the Y host is seriously weakened if Kondo pair-breaking is strong. We conclude that pressure-enhanced Kondo binding is indeed responsible for the volume collapse in Pr, whereas in Gd simple s − d electron transfer is the appropriate mechanism.

1Work at Washington University is supported by NSF grant DMR-1104742 and CDAC through NNSA/DOE grant DE-FC52-08NA28554. Work at the Argonne Labs is supported by DOE contract DE-AC-02-06CH11357.
M1.0017 High-pressure synthesis of BiFeO$_3$-BiAlO$_3$ and BiFeO$_3$-MnTiO$_3$ solid solution. GEN SHIMURA, KEIJI KUSABA, TETSUYA MIYAWAKI, KEN NIWA, HIDEFUMI ASANO, MASASHI HASEGAWA, Nagoya University — There have been so many investigations for high-pressure synthesis of perovskite-type oxides in the material science field. Multiferroic material is particularly attracted in the field of electronic device materials. BiFeO$_3$ (ferroelectric antiferromagnet) is known as the only Bi-contained perovskite which can be synthesized at ambient pressure. We investigated solid solution systems of BiFeO$_3$-BiAlO$_3$ and BiFeO$_3$-MnTiO$_3$ under high pressure and high temperature to synthesize a new multiferroic compound in the present study. Chemical reagents of simple oxides were mixed with a mortar as a starting material. The mixture was raped with a gold foil, and it encased in a cubic press-medium with a graphite furnace. High pressure experiments were carried out using two DIA-type high pressure apparatuses installed in Nagoya University. X-ray powder diffraction patterns of all recovered specimens were collected using Cu-K$_\alpha$ radiation and magnetic susceptibilities for some of the recovered specimens were measured using a vibrating sample magnetometer. In the system of BiFeO$_3$-BiAlO$_3$, the BiFeO$_3$-type solid solution was only obtained in the both Fe- and Al-rich composition. While in the system of BiFeO$_3$-MnTiO$_3$, no solid solutions were observed.

M1.0018 High pressure x-ray diffraction and Raman spectra study of V$_2$O$_3$. LIGANG BAI, MICHAEL PRAVICA, YUSHENG ZHAO, Department of Physics and Astronomy, University of Nevada Las Vegas and High Pressure Science and Engineering Center (HIPSEC), Las Vegas, NV 89154, SERENA CORR, School of Chemistry, University of Glasgow, Glasgow, Scotland, YANG DING, The Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA, STAS V. SINOEIKIN, YUE MENG, CHANGYONG PARK, GUOYIN SHEN, High Pressure Collaborative Access Team, Geophysical Laboratory, Carnegie Institution of Washington, Argonne, IL 60439 USA — The structural and vibrational properties of V$_2$O$_3$ have been investigated on basis of synchrotron x-ray diffraction and Raman scattering in a diamond anvil cell. The structure analysis based on the Rietveld refinement methods shows the pressure dependence of V-O and V-V bonding distances. The compressibility of volume and cell axis under different pressure medium is discussed. The pressure dependence of Raman modes was obtained and compared with the existing low temperature measurements. A new high pressure phase of V$_2$O$_3$ was observed by x-ray diffraction and also predicted by ab initio method. This new phase has similar structure with low temperature phase.

M1.0019 The effect of high pressure on the density and viscosity of liquid sulfur. KEN-ICHI FUNAKOSHI, AKIFUMI NOZAWA, Japan Synchrotron Radiation Research Institute, SPring-8 — Liquid sulfur has attracted attention because it is a complex system that exhibits anomalous properties such as density and viscosity with changes in temperature and pressure. Brazhkin et al. (1991) suggested a first-order liquid-liquid phase transition of liquid sulfur occurs at pressure around 8 GPa. However, no dramatic change accompanying the phase transition has been observed in the previous high pressure viscosity experiment, and this transition is still under debate (Terasaki et al. 2004). Recently, we designed a new method for measuring the density and viscosity of liquid at high pressure using synchrotron radiation and a multi-anvil press (Funakoshi et al. 2012). We successfully obtained the density and viscosity of liquid sulfur and determined the precise compression curve at pressures up to 11 GPa. The density of liquid sulfur showed a smoothly increase and no sharp changes with increasing pressure. This behavior indicates that the long polymeric chain structure of liquid sulfur is continuously compressed after the λ-transition. However, an abrupt increase in the viscosity was observed around 9 GPa. This remarkable change in the viscosity suggests that a second-order phase transition without structural changes may have occurred in the pressure range.

M1.0020 Phase Transitions and Melting in Magnesium to 200 GPa and 4500 K. S. STINTON, The University of Edinburgh, Edinburgh, UK, S. MACLEOD, The Atomic Weapons Establishment, Aldermaston, UK, H. CYN, Lawrence Livermore National Laboratory, Livermore, CA, USA, D. ERRANDONEA, Universitat de Valencia, Valencia, Spain, J. PROCTOR, The University of Edinburgh, Edinburgh, UK, Y. MENG, Geophysical Laboratory, Carnegie Institution of Washington D.C., USA, M. MCMAHON, The University of Edinburgh, Edinburgh, UK — Magnesium is a “simple” nearly free-electron metal up to around 100 GPa. Despite similarly-simple group II metals being the subject of numerous studies that have revealed complex high-pressure behaviour, Mg has very few high-pressure diffraction studies, particularly above room temperature. Here we describe such studies to above 200 GPa at 300 K, combined with resistive- and laser-heating experiments to 4500 K and 100 GPa. The dhcp-bcc transition at ~50 GPa exhibits a large region of phase co-existence at all temperatures up to 800 K, and the transition pressure is found to decrease with temperature at the rate of ~3.4 GPa per 100 K, somewhat smaller than the rate calculated by Mehta et al. [1]. At lower pressures, below the melting curve at 10 GPa, we find the dhcp phase to be stable, in agreement with Errandonea et al. [2]. Laser heating studies to 4500 K and 100 GPa show that Mg remains dhcp up to the melting curve, our measurement of which is in good agreement with the previous “speckle” studies of Errandonea et al. [3]. [1] S. Mehta, et al., J. Chem. Phys. 125, 194507 (2006). [2] D. Errandonea, et al., J. Phys.: Condens. Matter 15 (2003) 1277–1289 [3] D. Errandonea, et al. Phys. Rev. B 65, 012108 (2001)

M1.0021 Angle-Distortion Equations in Special Relativity. FLORENTIN SMARANDACHE, The University of New Mexico — Let’s consider an object of triangular form $\Delta ABC$ moving in the direction of its bottom base $BC$ (on the $x-$axis), with speed $v$. The side $|BC|=\alpha$ is contracted with the Lorentz contraction factor $C(v) = \sqrt{1-v^2/c^2}$ since $BC$ is moving along the motion direction, therefore $|B'C'|=\alpha C(v)$. But the oblique sides $AB$ and $CA$ are contracted respectively with the oblique-contraction factors $OC(v, B)$ and $OC(v, \pi-C)$, where the oblique-length contraction factor is defined as:

$$OC(v, \theta) = \sqrt{C(v)^2 \cos^2 \theta + \sin^2 \theta}.$$ 

In the resulting triangle $\Delta A'B'C'$ one simply applies the Law of Cosine in order to find each distorted angle $A'$, $B'$, and $C'$. Therefore:

$$A' = \arccos \left( \frac{-\alpha^2 \cdot C(v)^2 + \beta^2 \cdot OC(v, A+B)^2 + \gamma^2 \cdot OC(v, B)^2}{2 \alpha \cdot \gamma \cdot OC(v, B) \cdot OC(v, A+B)} \right),$$

$$B' = \arccos \left( \frac{\alpha^2 \cdot C(v)^2 - \beta^2 \cdot OC(v, A+B)^2 + \gamma^2 \cdot OC(v, B)^2}{2 \alpha \cdot \gamma \cdot OC(v, B) \cdot OC(v, A+B)} \right),$$

$$C' = \arccos \left( \frac{\alpha^2 \cdot C(v)^2 + \beta^2 \cdot OC(v, A+B)^2 - \gamma^2 \cdot OC(v, B)^2}{2 \alpha \cdot \beta \cdot C(v) \cdot OC(v, A+B)} \right).$$

The angles $A'$, $B'$, and $C'$ are, in general, different from the original angles $A$, $B$, and $C$ respectively. The distortion of an angle is, in general, different from the distortion of another angle.
M1.00022 Gahnite under high pressure: A XRD insitu study. CHRISTIAN LATHE, Helmholtz Centre Potsdam GFZ German Research Centre for Geosciences, Potsdam, Germany; MICHAEL PETER, CHRISTIAN LATHE, Helmholtz Centre Potsdam GFZ German Research Centre for Geosciences, Potsdam, Germany — Placing P-T-t constraints on planetary differentiation Natural gahnite has the ideal formula ZnAl$_2$O$_4$. Together with franklinite (ZnFe$_2$O$_4$) it forms a limited solid solution at high temperatures an occurs as an accessory phase in magmatic and metamorphic rocks, but mainly in the Franklin marble and skarn deposits (Carvalho and Sclair 1988, Froendt and Grom 1991). A natural gahnite sample was investigated with large volume presses at the Synchrotron source DESY. Pressure was stepwise increased to 5 GPa at the MAX08 and 15 GPa at MAX300v and diffraction patterns were collected after each step. The determined volume-pressure-data are fitted to a 2nd and 3rd order Birch–Murnaghan equation of state to obtain the isothermal bulk modulus $K_{02nd}$ and its pressure derivative $K'$. Isothermal bulk modulus was derived from XRD data. Using a 2nd and 3rd order Birch-Murnaghan equation of state revealed $K_{02nd} = 207(4)$ GPa and $K' = 4.9(3)$, respectively. A significant change of the pressure derivatives of C11, C12 and C44 at a pressure of approximately 15 GPa indicates a 2nd order phase transition in gahnite.

M1.00023 Determination of Equations of State for AlF$_3$ and AlI$_3$: Semi-empirical Modeling of Extreme Condition Halide Chemistry. J. JOSEPH ZAUG, Lawrence Livermore National Laboratory, ELISSAIOS STAVROU, Carnegie Institute of Washington, SOVIN BASTEA, Lawrence Livermore National Laboratory, ALEXANDER GONCHAROV, Carnegie Institute of Washington, JONATHON CROWHURST, SARAH ROBERTS, JONATHAN PLAUE, Lawrence Livermore National Laboratory, JEFFREY CARTER, picarro.com, MICHAEL ARMSTRONG, Lawrence Livermore National Laboratory — Pressure dependent angle-dispersive x-ray powder diffraction measurements of alpha-phase aluminum trifluoride (alpha-AlF$_3$) and separately, aluminum triiodide (AlI$_3$) were conducted using a diamond- anvil cell. Results at 295 K extend to 50 GPa. The equations of state of AlF$_3$ and AlI$_3$ were determined through refinements of collected x-ray patterns. The respective bulk moduli and corresponding pressure derivatives using multiple orders of the Birch-Murnaghan, Ff, and Gg EoS models will be discussed. Aluminum trifluoride exhibits no pressure induced structural phase transition, while the triiodide data reveal a second-order is-structural rearrangement. Applied stress transformed a monoclinically distorted face-centered cubic (FCC) structure into a perfect FCC structure. Results from semi-empirical thermochemical computations of energetic materials formulated with fluorine containing reagents will be presented.

M1.00024 In situ high-pressure-temperature synchrotron XRD study of Mo with laser-heated diamond anvil cells. QIANG ZHOU, XIAOLI HUANG, FANGFEI LI, BINGBING LIU, TIAN CUI, National Lab of Superhard Materials, YUE MENG, HPCAT, APS, NATIONAL LAB OF SUPERHARD MATERIALS COLLABORATION, HPCAT, APS COLLABORATION — In order to understand the behavior of materials at high pressure and high temperature, it is important to have a precise knowledge of pressure (P) - volume (V) - temperature (T) relationship. In this paper, Mo is studied by an integrated technique of diamond anvil cell, laser-heated and synchrotron XRD technologies, providing experimental insight into its behavior at high pressure and temperature. We have measured the cold compression of Mo with the neon pressure media up to 77 GPa, and its thermal expansion up to 94 GPa and 3470 K. The third-order Birch–Murnaghan EoS of Mo at room temperature can be fitted with $K_{0} = 267$ GPa, $K_{0}' = 3.4$, with $V_0 = 31.32$ A$^3$. High temperature data have been treated with both thermodynamic and Mie–Grüneisen-Debye methods for the thermal EoS inversion. The results are self-consistent and in agreement with those obtained by previous theoretical data. The crystal structure of Mo is determined up to 94 GPa and 3470 K and no evidence for the predicted transition to a close-packed face-centered cubic (fcc) phase is found.

M1.00025 Properties of high density gaseous nitrogen under shock compression in hemispherical geometry. MIKHAIL ZHERNOCKLETOV, SERGEI KIRSHANOV, ALEXEI KOVALEV, ALEXANDER MEZHEVOV, MIKHAIL NOVIKOV, RFNC-VNIIEF — Recent investigations of liquid nitrogen properties under shock compression show compressive limit of 4.2 close to that of ideal gas $\sigma = 4$ in pressure region 100 – 330 GPa and demonstrate an unusual Hugoniot pressure – density dependence similar to isochoric compression. We performed two experiments with gaseous nitrogen with initial density $\rho_0 = 0.8$ g/cm$^3$ to confirm previous data on liquid nitrogen. The experiments were conducted using HE shock wave generators of hemispherical geometry. We obtain Hugoniot pressures (190 ± 5) and (226 ± 5) GPa, compressions (4,64 ± 0,47) and (4,42 ± 0,36), temperatures (37500 ± 5800) and (45900 ± 9300) K. Experimental data on gaseous nitrogen agree with that on liquid nitrogen and modified model of compressible covolume.

M1.00026 ABSTRACT WITHDRAWN —

M1.00027 Equations of state for hydrocodes. I.V. LOMONOSOV, IPCP RAS — The equation of state (EOS) governing the system of gas dynamic equations defines significantly accuracy and reliability of results of numerical modeling. In our report, we will formulate main mathematical and physical demands to wide-range EOS for hydrocodes. Our semi-empirical EOS model fully assigns the free energy thermodynamic potential for metals over entire phase diagram region of practical interest. It accounts for solid, liquid, plasma states as well as two-phase regions of melting and evaporation. Available now are wide-range multi-phase EOS for 30 simple and transition metals of the most practical interest. Their direct usage in computer codes leads to complicated and not economy calculations, so they are usually involved in numerical simulating in tabular form. The EOS code for calculation of tables can produce the complete set of thermodynamic derivatives (such as pressure, sound velocity, heat capacity) using any of input pairs: volume-temperature, volume-internal energy or volume-pressure. The input grid can be linear, logarithmic or arbitrary; each point in 2D output tables is marked by symbol which indicates the physical state, such as solid, liquid, gas, plasma or mesh. We also present in our talk estimations of shock melting and evaporating and importance of these effects for results of numerical modeling.

M1.00028 Reversible pressure-induced polymerization of C$_{60}$/C$_{70}$ doped ferrocene. WEN CUI, MINGGUANG YAO, QUANJUN LI, RAN LIU, BO LIU, ZHEN YAO, FENGXIAN MA, BINGBING LIU, Jilin University — C$_{60}$/C$_{70}$ combined with organometallic donors can form a wide variety of donor-acceptor complexes and only relatively weak van der Waals interactions and charge transfer between them. Ferrocene (Fc) is an example with the tunable degree of charge transfer to C$_{60}$/C$_{70}$ and offers us a good model to study the effect of charge transfer on the polymerization of fullerene. Pressure can modify the intermolecular distance and thus affect the charge transfer between host and guest. It is expected that the interaction can be tuned by applying pressure and further affect the polymerization of fullerene. In situ high pressure Raman, IR and XRD studies are used to investigate the phase transitions of C$_{60}$/C$_{70}$(Fc)$_2$. We find that the charge transfer interaction is strengthened under pressure and the polymer chain is formed in C$_{60}$(Fc)$_2$ at 5GPa, while dimer phase and 1D/2D polymers are formed in C$_{70}$(Fc)$_2$ at 3GPa and at 8GPa, respectively. Only certain fullerene molecules take part in this reaction due to the layered structure of the samples. These transitions are quite different from those of pure C$_{60}$/C$_{70}$ because of the intercalated Fc. The observed polymerization is reversible and can be related to the overriden steric repulsion of counter ions and the tunable charge transfer at high pressure.
**M1.00029 High pressure study of RNi intermetallics (R=Dy, Gd)**, POOJA RANA, UDAI PRATAP VERMA, School of Studies in Physics, Jiwaji University, Gwalior — The structural, electronic and magnetic properties of RNi’s (R=Dy, Gd) have been analyzed using \textit{ab-initio} full-potential linear augmented plane wave method within the density functional formalism. Spin polarized GGA+U approximations based on exchange-correlation energy optimization has been used for the calculation of total energy of the systems. Under compression, DyNi undergoes a first-order structural phase transformation from ambient FeB to CsCl phase at 18.4 GPa while GdNi transform its structure from CrB to CsCl phase at 3.73 GPa. The calculated magnetic moment for R$^{3+}$ ions are obtained as 9.3 $\mu_B$ and 7 $\mu_B$, respectively, in DyNi and GdNi. The results are closer to the experimental values (10 $\mu_B$ for Dy$^{3+}$ and 7 $\mu_B$ for Gd$^{3+}$). Details related to structural, electronic and magnetic properties are reported, theoretically, for the first time for DyNi intermetallic compound. The equilibrium lattice constants are in good agreement with their experimental data. Our calculation shows that both the intermetallic compounds are metallic in nature.

**M1.00030 ABSTRACT WITHDRAWN**

**M1.00031 Phase Decomposition of Rare Earth Apatite and Formation of Perovskite Rare Earth Silicate at High Pressure and High Temperature Conditions**, FUJXIAN ZHANG, MAIK LANG, RODNEY EWING, University of Michigan — The crystal structure of rare earth apatite was studied at high pressure and room temperature conditions. A reversible sublattice phase transition was found at pressure. The high-pressure phase has also a hexagonal unit cell but with a lower symmetry reduced from P6$_3$/m to P6$_3$. Due to the symmetry change, the high-pressure phase has an unusual lower bulk modulus as compared with the corresponding ambient structure. Laser heating of La-Si-O apatite at high pressure conditions revealed that apatite structure is not stable at temperatures higher than 1500 K and decomposes into two different phases. The decomposed phase is a perovskite-type structure. Alkaline earth silicate minerals can easily form the 6-coordinated high-pressure phase in the deep earth environment. However, a rare earth silicate with the perovskite structure has not been previously reported. The experimental results also suggest that the La$_{0.67}$SiO$_3$ perovskite structure is at least partially quenchable.

1This work was supported by Materials Science of Actinides, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award No. DE-SC0001089.

**M1.00032 High energy-resolution electron energy-loss spectroscopy and x-ray emission spectroscopy studies of amorphous diamond transformed from neutron-irradiated graphite**, YOHEI SATO, MASAMI TERAUCHI, Tohoku University, KEISUKE NIWAISE, Hyogo University of Teacher Education, KAZUTAKA G. NAKAMURA, TOSHIYUKI ATOU, Tokyo Institute of Technology, TADAOWA I, University of Tokyo — Specimens for transmission electron microscopy were prepared from amorphous diamond, which was synthesized from neutron-irradiated graphite by shock compression. High energy resolution EELS measurements were performed by using a monochromator transmission electron microscope (TEM). XES measurements were performed by using a wavelength-dispersive-type spectrometer for soft x-ray attached to the monochromator TEM. A volume plasmon peak of am-DIA is observed at 32.5 eV, which is slightly located at lower energy than that of c-DIA. Since the plasmon energy is dominantly proportional to square root of valence electron density, the lower plasmon energy of am-DIA indicates that the valence electron density of am-DIA is smaller than that of c-DIA. Also, it is revealed that the band gap energy of am-DIA is 4.0 eV, which shows good agreement with the estimation of 3.9 eV from the onset energy of valence-electron excitation spectrum.

**M1.00033 Pressure-induced phase transition in $\gamma$-MnOOH**, WOLFGANG H. MORGENTROTH, BJORN WINKLER, Goethe-Universitaet Frankfurt, Altenhoeferallee 1, 60438 Frankfurt a.M., Germany, VICTOR MILMAN, Accelerx, 334 Science Park, Cambridge CB4 0WN, UK — At ambient conditions, $\gamma$-MnOOH, crystallizes in space group P2$_1$/c (Kohler et al. 1997). A high pressure study by Suzuki (2006) up to 9 GPa gave a bulk modulus of 91(2) GPa, when the data was fitted with a 2$^{\text{nd}}$ order Birch-Murnaghan equation of state. Preliminary DFT calculation predicted a phase transition to an orthorhombic space group at pressures above 15 GPa. In order to test the prediction, natural $\gamma$-MnOOH was ground to powder and compressed in a DAC up to 70 GPa. Lattice parameters were determined from X-ray patterns recorded at the Extreme Conditions Beamline P02.20PETRA III. A structural phase transition into an orthorhombic phase was observed at 47 GPa. The bulk modulus of the ambient pressure phase is 98(3) GPa with $K'_0=7.7(3)$. Currently, DFT+U calculations are carried out to understand the compression mechanism and the phase transition. Funding by the BMBF (project 05K10RFA) is gratefully acknowledged. We thank DESY Photon Science for beam time and Hanns-Peter Liermann and his team for support. Kohler T. et al., J Solid State Chemistry, 1997, 133, 486-500. Suzuki A., SPring-8 Exp. Report, 2006, 2006A1464.

**M1.00034 Molybdenum Sound Velocity and Shear Strength Softening**1, JEFFREY NGUYEN, MINTA AKIN, RICKY CHAU, DAVEY FRATANDOUNO, PAT AMBROSE, Lawrence Livermore National Laboratory, OLEG FATYANOV, PAUL ASIMOW, California Institute of Technology, NEIL HOLMES, Lawrence Livermore National Laboratory — We recently carried out a series of light-gas gun experiments to measure molybdenum acoustic sound speed up to 5 Mbars on the Hugoniot. Our measured sound speeds increase linearly with pressure up to 2.6 Mbars and taper off near the melting pressure. The gradual leveling off of sound speed suggests a possible loss of shear strength near the melt. A linear extrapolation of our data to zero pressure is in good agreement with the sound speed measured at ambient condition. The results indicate that molybdenum remains in the bcc phase on the Hugoniot up to the melting pressure. There is no bcc solid phase transition on the Hugoniot as previously reported.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

**M1.00035 Bcc-fcc structure transition of Te**, TOSHIYUKI SUGIMOTO, YUICHI AKAHAMA, TOMOHIRO ICHIKAWA, Graduate School of Material Science, University of Hyogo, HIROSHI FUJIHISA, Graduate School of Material Science, University of Hyogo, HIROSHI FUJIHISA, National Institute of Advanced Industrial Science and Technology, NAOHISA HIRAO, YASUO OHISHI, Japan Synchrotron Radiation Research Institute — A group 16 element, tellurium (Te) undergoes numerous structural phase transitions at pressure up to 255 GPa and at room temperature have been carried out and the bcc-fcc structure transition is reported.

**M1.00036 Electrical properties (ZrO$_2$+Y$_2$O$_3$+Al$_2$O$_3$) at high pressures**, ANNA TREFILOVA, ALEXEY BABUSHKIN, YULIA SEMENOVA, Ural Federal University — We studied electrical resistance (ZrO$_2$+Y$_2$O$_3$+Al$_2$O$_3$) at the pressures 22 - 50 GPa and temperatures 77 - 400 K. Measurements were made with samples containing 80% (ZrO$_2$+3mol%Y$_2$O$_3$+20%Al$_2$O$_3$). The d.c. conductivity measurements were carried out in a diamond anvil cell (DAC) with anvils of the “rounded cone-plane” (Verechagin–Yakovlev) type made of synthetic carbonado-type diamonds, consisting of dielectric grains of synthetic diamonds in layers of conducting materials. These anvils are relatively good conductors, thus permitting measurement of the resistances of samples placed between the anvils in the DAC by using the anvils as the electrical contacts to the sample At a pressures of about 28-30 GPa the (ZrO$_2$+Y$_2$O$_3$+Al$_2$O$_3$) resistance decreases by 3-4 orders of magnitude. The temperature dependences of the resistance exhibit a metal-like character (with the positive temperature coefficient).
M1.00037 High Pressure Raman and X-ray diffraction studies on MoS2 up to 51 GPa. JASON BAKER, RAVHI KUMAR, NIRUP BANDARU, DANIEL ANTONIO, RAMA VENIKAT, THOMAS HARTMANN, DANIEL SNEED, YUSHENG ZHAO, University of Nevada, Las Vegas — Molybdenum disulfide (MoS2) is technologically important material which finds potential applications as high temperature lubricant, universal joint in ultra high vacuum chambers and in photovoltaic devices. Recent studies show excellent antishock or shock-absorbing property under very high shock wave pressures of 25 GPa and temperature up to 1,000°C. We have investigated the structural stability of MoS2 under high pressure conditions up to 51 GPa using synchrotron x-ray diffraction (XRD) in an angle dispersive geometry and a diamond anvil cell using Ne pressure medium. Raman spectra were collected up to 30 GPa. Furthermore, we have also performed high temperature x-ray diffraction up to 450°C at ambient pressure conditions. Analysis of both XRD and Raman data indicate a pressure induced phase transition occurring above 20 GPa from the ambient hexagonal to a possible high pressure orthorhombic phase. The results will be presented in detail.

M1.00038 Coupling of strong elastic shock with supersonic melting front produced by ultra-short laser pulse. NAIL INOGAMOV, Landau Institute for Theoretical Physics of RAS, VASILIY ZHAKHOVSKY, BRIAN DEMASKE, University of South Florida, VIKTOR KHOKHLOV, Landau Institute for Theoretical Physics of RAS, IVAN OLEYNIK, University of South Florida — Generation of ultra-short shock elastic and plastic waves by femtosecond laser pulses in Al and Ni films is investigated by two-temperature hydrodynamics (2T-HD) and molecular dynamics (MD) methods. Ultrafast laser heating of metals is approximately isochoric during first several picoseconds. It leads to significant overheating of surface layer above the equilibrium melting line $T_m(P)$, causing the melting front to propagate with supersonic speed as deep as a local degree of overheating drops to ~1.2. After that the melting front decelerates quickly and a compression wave leaves the heated surface layer. Because the melting transition occurs at isochoric compression, the pressure and temperature at a solid-liquid interface in a moment when the melting front stops are independent on laser energy absorbed in metals. If absorbed energy exceeds some threshold, the compression wave splits into elastic and plastic shock waves. Evolution of those waves, including their coupling with the melting front at early stage and emission of rarefaction and compression elastic pulses by a plastic front, was studied by both 2T-HD and MD simulation. It was shown that the elastic precursor has a fluence-independent amplitude; whereas the plastic front undergoes significant attenuation during propagation and may fully decay within a metal film.

M1.00039 Structural and superconducting properties of Bi$_{1-x}$Sb$_x$ under high pressure. AYAKO OHMURA, Center for Transdisciplinary Research, Niigata University, YASUSHI FUJIIKAWA, AYAKO YAMAMURA, MARI EI NAGA, Graduate school of Science and Technology, Niigata University, ATSUKO NAKAYAMA, Center for Transdisciplinary Research, Niigata University, FUMIHIRO ISHIKAWA, YUH YAMADA, Department of Physics, Niigata University, SATOSHI NAKANO, National Institute for Materials Science — We have studied pressure-induced superconductivity and structural phase transition in bismuth-antimony alloy (Bi$_{1-x}$Sb$_x$), which is a substitutional solid solution over the full composition range. Bi$_{1-x}$Sb$_x$ crystallizes in the A7-structure with space-group $I\bar{3}m$ at ambient condition and shows pressure-induced structural changes similar to those of pure Bi and Sb: the A7-structure – the incommensurate host-guest composite structure with super space-group $I\bar{4}/mcm(001)$ (the HP-composite phase) – the body-centered cubic one with $I\bar{3}m$ (bcc). In the composition of $x = 0.08$, these two phase transitions occur above 3 and 10 GPa, respectively. In pure Bi and Sb, the superconductivity is observed in these high-pressure phases. To investigate the superconducting transition in $x = 0.08$, we performed the electrical resistivity measurement at low pressure up to 12 GPa using modified Bridgman anvil cell. The superconducting transition is observed above 2.7 GPa with the transition temperature $T_c = 7.0$ K. Furthermore, $T_c$ discontinuously increases up to 8.5 K at 9.7 GPa. As compared to the structural change, the superconductivities observed at 2.7 and 9.7 GPa are attributed to the HP-composite structure and bcc, respectively.

M1.00040 Phase changes induced by guest ordering of filled ice Ih structure of methane hydrate under high pressure and low temperature. HISAHI HIRAI, TAKEHIKO TANAKA, Geodynamics Research Center, Ehime University, TAKAHIRO MATSUOKA, KYOKUGEN, Osaka University, YASUSHI TACHISHI, Japan Synchrotron Radiation Research Institute, TAKEHIKO YAGI, SHINGO KAGAWA, Geodynamics Research Center, Ehime University, MICHIKO OHTAKE, YOSHITAKA YAMAMOTO, The National Institute of Advanced Industrial Science and Technology — Orbital ordering of guest methane molecules in a filled ice Ih structure of methane hydrate (MH-FIIhS) was observed above 20GPa by our previous Raman study, whereas change in a fundamental structure was not detected by XRD. In this study, in-situ XRD studies were performed in the temperature range from 300 to 70 K at the pressures up to 57 GPa. The results revealed that the lattice parameters changed continuously with increasing pressure, however, clear changes in axes ratios were shown. At about 20 GPa the slopes of axis ratios, b/c and c/a, changed abruptly at room temperature. The Raman spectroscopy showed split of CH vibration mode of the methane molecules, which indicates the orientational ordering of the guest methane molecules, at the almost same pressure. These results demonstrated that the changes in axis ratio were caused by orientational ordering of the guest molecules. Similar changes in the axis ratios and split of CH vibration mode were observed at low temperature regions. The regions of the guest-ordered phase and the guest-rotated phase were roughly estimated from the experimental results.

M1.00041 Sound velocity determination of PbTe under pressure. MATTHEW JACOBSEN, School of Engineering and Centre for Science at Extreme Conditions, University of Edinburgh, United Kingdom, WEI LIU, BAOSHENG LI, Mineral Physics Institute and Department of Geoscience, Stony Brook University, New York, USA — Recent investigation of PbTe have revealed interesting high pressure transitions resulting in improved thermoelectric performance. High pressure sound velocities of PbTe have been measured to 14 GPa using an ultrasonic interferometric method. Elastic moduli and their pressure derivatives for phases in this range have been obtained using a finite strain approach. From this, an estimate of the acoustic phonon contribution to the thermal conductivity is made. By combining this with previous determinations of the thermal conductivity due to electrons, a significantly lower value than the previously determined total thermal conductivity is found. This is interpreted as evidence for coupling between the low-lying transverse optic (TO) and longitudinal acoustic (LA) modes allowing transfer of thermal energy between them. The application of pressure causes energy transfer between the optical modes and electron population, which is likely the cause of the increased thermoelectric efficiency in the intermediate PbTe phase.

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M1.00042 Study of electric properties of amorphous AgGe$_{1+x}$As$_{1-x}$S$_3$ with content of carbon nanotubes$^1$, NINA MELNIKOVA, KIRILL KUROCHKA, YANA VOLKOVA, UrFU — Multicomponent copper and silver chalcogenides have been known as promising materials for scientific and applied purposes. These materials are also under intense investigation for application in a phase-change random access memory$^1$. In order to obtain materials with a high ionic conductivity component, glassy silver chalcogenides AgGe$_{1+x}$As$_{1-x}$S$_3$ with the addition of nanotubes were synthesized. In this work the study of electrical properties of the amorphous chalcogenide AgGe$_{1+x}$As$_{0.6}$S$_3$ $(x = 0.4)$ with carbon nanotube content at a frequency of the alternating-current electric field varying from 1 Hz to 5 MHz and on direct current at ambient pressure and at pressure up to 30 GPa are presented. The ion transport was confirmed by means DC measurements in cells with blocking ion component of conductivity electrodes. An evaluation of the proportion of ionic conductivity can make a preliminary conclusion that the ionic component of the conductivity of at least 98%. Analyze of the basic dependences of AC properties have shown that the dielectric loss tangent and the real part of an admittance of the AgGe$_{1+x}$As$_{0.6}$S$_3$ with carbon nanotube content compound exponentially increase with a pressure increase from 1 up to 30 GPa.

$^1$The study was supported in part by the Ural Federal University development program with the financial support of young scientists; and by the Russian Foundation for Basic Research, project No. 12-02-31007.

M1.00043 Pressure effects on superconductivity in LaFeAsO$_1$-$\delta$ , FUMIHIRO ISHIKAWA, Department of Physics, Niigata University, MICHIIKO KODAMA, NAOYA EGUCHI, Graduate School of Science and Technology, Niigata University, AYAKO OHMURA, ATSUKO NAKAYAMA, Center for Transdisciplinary Research, Niigata University, YUH YAMADA, Department of Physics, Niigata University — Pressure effects on superconductivity in LaFeAsO$_1$-$\delta$ oxypnictide were studied using piston-cylinder type pressure cell. LaFeAsO$_1$-$\delta$ has been recognized as one of the typical FeAs-based superconductor since the discovery of superconductivity in LaFeAs(O, F). Oxygen deficiency in LaFeAsO leads doping and causes superconductivity. Pressure dependence of the superconducting transition temperature of LaFeAsO$_1$-$\delta$ was clarified by electrical resistivity measurement up to the pressure of $P = 2.5$ GPa. The sample of LaFeAsO$_1$-$\delta$ was prepared by high pressure synthesis technique. Using a cubic-anvil-type apparatus the sample was sintered at 1250°C under the pressure of 3 GPa. Oxygen deficiency was estimated from the nominal composition of starting materials. At ambient pressure, LaFeAsO$_1$-$\delta$ shows superconducting transition at $T_c = 21.8$. With increasing pressure, $T_c$ increased almost linearly with coefficient of $dT_c/dP = 2.6$ K/GPa. The pressure dependence of $T_c$ in LaFeAsO$_1$-$\delta$ is similar to that of an under doped sample in the LaFeAs(O, F) system.

M1.00044 Pressure Effect on Superconductivity of Rhenium, KAZUSHI TAKAHAMA, TAKAHIRO MATSUOKA, KATSUYA SHIMIZU, KYOKUGEN, Osaka Univ., Japan — Rhenium metal is often used as a gasket material in high pressure experiments using DACs. It has been known that rhenium is a superconductor with superconducting transition temperature $T_c$ of 1.6-2.8 K at ambient pressure$^1$. Although, pressure dependence of $T_c$ has not been studied in detail over 2 GPa$^1$. It’s important to study pressure effect on $T_c$ of Re in two points. First is that simple elements Os, W, Ir and Re are known to superconduct with very low $T_c$ at ambient pressure, but high pressure properties of their $T_c$ have not been well studied so far. Another point is a technical aspect. In the studies of superconductivity under high pressures, we employ electrical resistance and magnetic susceptibility measurements to detect superconductivity. Superconducting Re-gasket below 4 K masks superconducting signal of sample in magnetic susceptibility measurements. In electrical resistance measurements, if the electric circuit has a short with Re-gasket, superconducting transition comes to be mixed in measured data. We present pressure dependence of $T_c$ of rhenium up to 65 GPa measured using a DAC. We observed $T_c$ increases in pressure range of 0-10 GPa and it gradually decreased with applied pressure.


M1.00045 Pressure-induced superconductivity in non-stoichiometric bismuth telluride Bi$_{2}$Te$_{0.5}$O$_{0.5}$, MARI EINAGA, Graduate School of Science and Technology, Niigata University, AYAKO OHMURA, Center for Transdisciplinary Research, Niigata University, FUMIHIRO ISHIKAWA, Department of Physics, Niigata University, SATOSHI NAKANO, AKIYUKI MATSUSHITA, NIMS, SHIGEKI TANAKA, TOMOKO KAGAYAMA, KYOKUGEN, Osaka University. — Stoichiometric bismuth telluride (Bi$_2$Te$_3$), which is a p-type semiconductor, has the rhombohedral structure with space group $R-3m$ at ambient condition. We have previously reported that pressure-induced superconductivity of stoichiometric type Bi$_2$Te$_3$ occurs in the high-pressure phases which appear above 8 GPa. The transport properties of Bi$_2$Te$_3$, however, depend on the atomic composition; the dominant charge carriers change from hole to electron above 63at.% Te. In this study, we performed the electrical resistivity measurement and the x-ray diffraction study of non-stoichiometric n-type Bi$_{2-x}$Te$_{0.5}$O$_{0.5}$ under high pressure to investigate pressure-induced superconductivity and structural phase transition. Bi$_{2.5}$Te$_{0.5}$O$_{0.5}$ has also the $R-3m$ structure at ambient condition. It remains stable up to 20 GPa at room temperature. The superconducting transition is observed at 6 GPa below 2.9 K. There is no obvious anomaly indicating structural phase transition in both pressure dependence of the electrical resistivity at pressures up to 65 GPa and temperature dependence of it at 6 GPa. It suggests that the superconducting transition at 6 GPa of Bi$_{2.5}$Te$_{0.5}$O$_{0.5}$ occurs in the $R-3m$ structure.

M1.00046 Parameterization of classical force fields in the context of high pressure calculations, BRANDON YANCiw, JEFFERY PERKINS, BRANDON WIEBE, University of the Fraser Valley, JACOB SPOONER, Simon Fraser University, NOHAM WEINBERG, University of the Fraser Valley, Simon Fraser University — Activation volumes and volume profiles of chemical reactions are concepts widely used in high pressure reaction kinetics. We have recently shown that these quantities can be calculated using molecular dynamics (MD) simulations with accuracy comparable to two of the experiment. The major challenge in performing such calculations comes from the fact that standard MD force fields are parameterized for stable species and, therefore, are not directly usable for transient points along the reaction coordinate. We propose a consistent scheme of parameterization for such species based on fitting force field potentials to quantum mechanical deformation energies, and show that MD simulations with these parameters produce molar volumes of quality comparable to that of OPLS and the experiment.

M1.00047 MD studies of electron transfer at ambient and elevated pressures, ALEX GILES, University of the Fraser Valley, JACOB SPOONER, Simon Fraser University, NOHAM WEINBERG, University of the Fraser Valley; Simon Fraser University — The effect of pressure on the rate constants of outer-sphere electron transfer reactions has often been described using the Marcus-Hush theory. This theory agrees well with experiment when internal reorganization of the ionic system is negligible however it does not offer a recipe for calculation of the effects that result from specific solute restructuring. We have recently developed a molecular dynamics technique that accurately describes structural dependence of molecular volumes in non-polar and weakly polar systems. We are now extending this approach to the case of highly polar ionic systems where both solvent and solute restructuring components are important. For this purpose we construct pressure-dependent two-dimensional surfaces for electron transfer reactions in coordinate system composed of interionic distance and Marcus-type solvent polarization coordinate, and use these surfaces to describe pressure effects on reaction kinetics.


M1.00048 Effect of high pressure on reaction profiles and energy surfaces. JACOB SPOONER, Simon Fraser University, BRANDON YANCZ, University of the Fraser Valley, NOHAM WEINBERG, University of the Fraser Valley; Simon Fraser University — Both experiment and first principles calculations unequivocally indicate that properties of elements and their compounds undergo a tremendous transformation at ultra-high pressures exceeding 100 GPa due to the fact that the difference between intra- and intermolecular interactions disappears under such conditions. Yet, even at much milder pressures of 5-30 GPa, when molecules still retain their individual identity, their chemical properties and reactivity change dramatically. Although first principles MD is perfectly suitable and, in fact, is being increasingly used to describe these systems, its applications are severely restricted by their size and complexity. Since, as long as transition state theory remains valid, the reaction kinetics and mechanisms can be described in terms of the free energy surfaces (FESs) of the solvated reaction systems, we propose to use classical molecular dynamics to describe effects of high pressure on condensed-phase FESs by calculating effects of solvation on the quantum mechanical gas-phase potential energy surfaces. We also show that high-pressure free energy surface $G(x)$ (x is a multidimensional geometrical parameter) is well approximated by equation $G(x) = G(0) + PV(x)$, where $G(0)$ is the zero-pressure free energy surface and $V(x)$ is the volume of reaction system in configuration $x$.

M1.00049 Structural and Vibrational Properties of Nitrogen-Hydrogen Mixtures at High Pressure. DYLAN SPAULDING, Harvard University, Cambridge, MA, 02138, GUNNAR WECK, PAUL LOUBEYRE, Commissariat a l’Energie Atomique, Bruyeres-le-Chatel, France, FREDERIC DATCHI, IMPMC, UPMC/Paris 6, Paris, France, PAUL DUMAS, Synchrotron SOLEIL, Gif-sur-Yvette, France, MICHAEL HANFLAND, European Synchrotron Radiation Facility, Grenoble, France — The chemistry and equations of state of simple molecular systems (e.g. N2, H2, CO2, CH4, C6H4 etc.) in the dense fluid state are of extreme importance to planetary astrophysics and are model systems for understanding the effects of pressure on chemical bonding, reactivity in the solid solution and potentially new routes to pressure-induced metallization. Here, we present the first comprehensive study of the binary N2/H2 system in the diamond anvil cell using Raman spectroscopy, synchrotron infrared micro-spectroscopy and visual observation. We find a eutectic-type binary phase diagram with two stable high-pressure compounds which we identify as (N2)6(H2)7 (R-3m) and N2(H2)2 (Pm-3m) using single-crystal x-ray diffraction. The former has a novel rhombohedral structure in which groups of hydrogen molecules are contained by the nitrogen lattice. We discuss further infrared absorption studies on this compound, including evidence for a gradual transformation from van der Waals to ionic interactions with pressure. A phase transition to an ionic compound with the same stoichiometry is observed at 55 GPa. Compression of this compound was carried out up to 200 GPa to investigate possible metallization.

M1.00050 High-pressure Brillouin study on plastic crystals of neopentane and adamantane. SHIGEO SASAKI, YASUHIRO HORIBE, TETSUJI KUME, Department of Materials Science and Technology, Gifu University — Spherical top molecules neopentane and adamantane withTd symmetry crystallize face centered cubic (fcc) plastic crystals in which molecules are rather freely rotating at fcc lattice points. In the case of fcc plastic crystalline methane, the value of elastic anisotropy $\lambda$ is above 5 which is large than $\lambda \sim 2.5$ of rare gas solids without molecular rotation, and shows strong pressure dependence because of the enhancement of the molecular rotation-translation (R-T) coupling by compression. Therefore, the purpose of the present study is to carry out the high-pressure Brillouin measurements for the fcc plastic crystals of neopentane and adamantane up to 0.75 and 0.5 GPa, respectively, and to clarify the dependence of the R-T coupling on pressure and molecular weight. The obtained value of $\lambda$ of fcc neopentane is 6.1 at 0.18 GPa and steeply increase up to 12.8 at 0.72 GPa. This remarkably large $\lambda$ values and its strong pressure dependence indicate that the R-T coupling effect in the plastic phase of neopentane is obviously large in comparison with methane. On the other hand, the plastic crystal of adamantane shows almost constant ($\lambda = 2.5$) which is nearly the same as the rare gas solids, suggesting no R-T coupling effect.

M1.00051 High-pressure Raman study of fully deuterated methane hydrate. RYO YABASHI, MASASHI YOSHIDA, TETSUJI KUME, SHIGEO SASAKI, Department of Materials Science and Technology, Gifu University — Methane hydrate (MH: CH4-nH2O) crystallizes in cubic phase I (Ih) in the dense fluid state. The cubic phase consists of hydrogen-bonded water cages which enclathrate methane molecules as guests. With increasing pressure, the initial sl of MH transforms to a hexagonal structure H (sh) at 0.9 GPa, and eventually to an orthorhombic cage-less structure O at 1.9 GPa. The sh consists of three small S1, two small S2, and one large LL water cages in a hexagonal unit cell. The previous high-pressure Raman measurements for C-H stretching vibration of MH-sH indicated that the capacity of methane molecules in the large LL cage abruptly increased at 1.3 GPa, and its occupation number consists of three small S1, two small S2, and one large LL water cages in a hexagonal unit cell. The previous high-pressure Raman measurements for the fcc plastic crystals of neopentane and adamantane up to 0.75 and 0.5 GPa, respectively, and to clarify the dependence of the R-T coupling on pressure and molecular weight. The obtained value of $\lambda$ of fcc neopentane is 6.1 at 0.18 GPa and steeply increase up to 12.8 at 0.72 GPa. This remarkably large $\lambda$ values and its strong pressure dependence indicate that the R-T coupling effect in the plastic phase of neopentane is obviously large in comparison with methane. On the other hand, the plastic crystal of adamantane shows almost constant ($\lambda = 2.5$) which is nearly the same as the rare gas solids, suggesting no R-T coupling effect.

M1.00052 Spectroscopic Studies of Cyclpentane under Extreme Conditions and Implications for the P-T Phase Diagram. CHUNLI MA, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road NW, Washington D.C. 20015, USA, QILIANG CUI, State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China, ROBERT C. LEGER, Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road NW, Washington D.C. 20015, USA — Infrared (IR) spectroscopy and Raman scattering combined with diamond anvil cell (DAC) and cryogenic techniques have been employed to investigate cyclpentane up to 4 GPa in the temperature range of 100-350 K and isothermal compression up to 84 GPA at room temperature. Four phases including liquid, plastic phases I and II, and truly crystalline phase III are clearly identified in the P-T range studied based on the changes of the ring breathing mode and CH2 rocking modes. The phase diagram is extended to the pressure and temperature range of 0 – 4.0 GPa and 105 – 350 K. Further compression at room temperature up to 84 GPA, another high-pressure phase (IV) is observed based on the appearance of low frequency peaks related to the lattice vibrational modes in the synchrotron far-IR spectra. The spectroscopic results indicate that cyclpentane persists the orientation ordered crystalline phase up to 84 GPA at room temperature.

M1.00053 Fe4O5: HP-HT synthesis and properties. SERGEY V. OVSYANNIKOV, Bayerisches Geoinstitut, Universität Bayreuth, Germany, ALEXANDER A. TSIRLIN, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, ALEXANDER E. KARKIN, VLADIMIR V. SHCHENNIKOV, Institute of Metal Physics, Russian Academy of Sciences, Yekaterinburg, Russia, ELENA BYKOVA, DMYTRO M. TROTS, ALEXANDER E. KARKIN, VLADIMIR V. SHCHENNIKOV, Institute of Metal Physics, Russian Academy of Sciences, Yekaterinburg, Russia, ALEXANDER A. TSIRLIN, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — Recently, a new iron oxide, Fe5O18 has been synthesized at high-pressure high-temperature (HP-HT) conditions [1,2]. In this work using multi-anvil large-volume cells we have investigated the synthesis conditions of Fe5O18 in wide pressures of 9-24 GPa and temperatures of 900-1800 C. We have prepared both single crystals and bulk polycrystalline samples of Fe5O18. We investigated the chemical composition and the microstructure of Fe5O18. From a single-crystal diffraction study we have established the crystal structure of Fe5O18. We have studied compressibility of Fe5O18 up to 50 GPa. In addition, we studied magnetic, optical and electronic transport properties of Fe5O18 at ambient pressure. These studies included magnetic susceptibility, magnetization, Mossbauer spectroscopy, Raman and Intra-red spectroscopy, electrical resistivity. We have performed also calculations of the lattice stability and electronic band structure of Fe5O18.


M1.00054 Effect of high pressure on reaction profiles and energy surfaces. JACOB SPOONER, Simon Fraser University, BRANDON YANCZ, University of the Fraser Valley, NOHAM WEINBERG, University of the Fraser Valley; Simon Fraser University — Both experiment and first principles calculations unequivocally indicate that properties of elements and their compounds undergo a tremendous transformation at ultra-high pressures exceeding 100 GPa due to the fact that the difference between intra- and intermolecular interactions disappears under such conditions. Yet, even at much milder pressures of 5-30 GPa, when molecules still retain their individual identity, their chemical properties and reactivity change dramatically. Although first principles MD is perfectly suitable and, in fact, is being increasingly used to describe these systems, its applications are severely restricted by their size and complexity. Since, as long as transition state theory remains valid, the reaction kinetics and mechanisms can be described in terms of the free energy surfaces (FESs) of the solvated reaction systems, we propose to use classical molecular dynamics to describe effects of high pressure on condensed-phase FESs by calculating effects of solvation on the quantum mechanical gas-phase potential energy surfaces. We also show that high-pressure free energy surface $G(x)$ (x is a multidimensional geometrical parameter) is well approximated by equation $G(x) = G(0) + PV(x)$, where $G(0)$ is the zero-pressure free energy surface and $V(x)$ is the volume of reaction system in configuration $x$.
M1.00054 Shear-induced phase transition of disordered nanocrystalline hexagonal boron nitride at room temperature\textsuperscript{1}. CHENG Ji\textsuperscript{2}, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA. VALERY LEVITAS, Department of Aerospace Engineering, Mechanical Engineering, and Material Science Engineering, Iowa State University, Ames, IA 50011, USA. HONGYANG ZHU, State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, Jilin, PR China. JHARNA CHAUDHURI, ARCHIS MARATHE, YANZHANG MA, Department of Mechanical Engineering, Texas Tech University, Lubbock, Texas 79409, USA. — Disordered hexagonal boron nitride (hBN) is an important precursor material for the synthesis of super-hard materials, wurtzitic BN (wBN) and cubic BN. However, the phase transformations from disordered hBN were only achieved at high temperatures under high pressures. By applying large shear by rotational diamond anvil cell, we observed the phase transition from disordered nanocrystalline hBN to wBN at room temperature under a moderate pressure of 6.7 GPa. Yet, under hydrostatic compression to 52.8 GPa, the same hBN sample did not transform to wBN. Our results demonstrate a potential of low pressure-room temperature synthesis of super-hard materials under plastic shear from disordered or amorphous precursors.

\textsuperscript{1}We acknowledge financial supports from Army Research Office and the Defense Threat Reduction Agency.

\textsuperscript{2}Also at High Pressure Synergetic Consortium, Carnegie Institution of Washington, Argonne, IL 60439, USA.

M1.00055 Pressure-induced structural transformations of 1D nanostructured TiO\textsubscript{2}. YANG SONG, ZHAOHUI DONG, ANKANG ZHAO, University of Western Ontario — Nanostructured materials especially semiconductors in different morphologies such as dots, wires, belts and tubes are of fundamental importance because of their wide range of tunable electrical, optical and mechanical properties. Investigations of the structures and phase transformations of nanomaterials under high pressures have received increasing attention. This is because, in addition to composition and synthetic routes, high pressure provides an additional effective driving force to produce new structures and, therefore, new nanomaterial properties. Using vibrational spectroscopy and synchrotron X-ray probes, in particular, we have studied several nanostructured TiO\textsubscript{2} materials under high pressure in situ to explore their high-pressure behaviors in terms of transformation pressures, phase stability regions and compressibility. Interestingly size dependent phase transitions were observed in all those nanomaterials comparing with the corresponding bulk materials.

M1.00056 High-pressure Phase Transition of Hexagonal Silver Sulfide Nano Platelets. RAN LIU, BINGBING LIU, QUANJUN LI, MINGGUANG YAO, BO LIU, HANG LV, SHUANGCHEN LIU, State Key Lab of Superhard Materials, Jilin University. JING LIU, Institute of High Energy Physics, Beijing, China. DONGMEI LI, BO ZOU, TIAN CUI, State Key Lab of Superhard Materials, Jilin University — Silver sulfide (Ag\textsubscript{2}S) is a narrow band gap semiconductor. Due to the excellent photoelectric and thermoelectric properties, silver sulfide has been widely used in the field of photocell, photoconductive devices and infrared detectors. Recent years, the discovery of fast ionic conductivity of silver sulfide at high temperature, making it become the research focus once again. Previous studies is limited to the temperature-induced phase transitions, the study of pressure-induced phase transition has not been reported. In order to study the pressure-induced phase transition properties of silver sulfide, the high-pressure synchrotron radiation XRD study on hexagonal silver sulfide nanoplates was carried out. Silver sulfide sample was in the morphology of regular hexagonal nanoplate, with an average diameter of 20nm. High-pressure synchrotron radiation XRD experiments shows that, under high-pressure, the diffraction peaks of silver sulfide are broadening. When the pressure reaches 12.4GPa, the sample transformed into amorphous state gradually and kept the amorphous state until the end of experiment, the highest attainable pressure was 29.4GPa. After the sample quenched to the initial pressure, it returned to the initial monoclinic \(\alpha\)-Ag\textsubscript{2}S phase, phase transformation was reversible.

M1.00057 Superconductivity of Mg/MgO interface formed by shock-wave pressure\textsuperscript{1}. V. AVDONIN, D. SHAKHRAY, Institute of Problems of Chemical Physics RAS, Chernogolovka, A. PALNICHENKO, N. SIDOROV, O. VYASELEV, S. KHASANOV, Institute of Solid State Physics RAS, Chernogolovka — Instability of the non-equilibrium superconducting Mg/MgO-interface under normal conditions has motivated our attempt to create it using shock-wave pressure. During the shock-wave impact, a stroke applied to the sample creates a series of strong high-pressure shock-waves propagating throughout the sample due to relative displacements of local parts of the sample material. Highly non-equilibrium conditions thus realized, can stimulate phase transitions or mechanochemical reactions inaccessible in a static pressure mode. Furthermore, the energy of the shock wave rapidly propagating through the sample within 10\textsuperscript{−6} – 10\textsuperscript{−9} s, leads to local non-equilibrium overheat of the sample’s regions at the shock wavefront, followed by their rapid cooling (quenching) as the shock-wave is passed. Such quenching can provide room-temperature stabilization of metastable non-equilibrium phases, unstable otherwise under normal conditions. A mixture of Mg and MgO has been subjected to a shock-wave pressure of \(\leq 20\) GPa. The ac susceptibility measurements of the product has revealed a metastable superconductivity with \(T_C \approx 30\) K. Comparison of the ac susceptibility and the dc magnetization measurements infers that the superconductivity arises within the interfacial layer formed between metallic Mg and its oxide due to the shock-wave.

\textsuperscript{1}This study was supported by RFBR, the grant N 13-02-01217A.

M1.00058 Regenerated Spider Silk Possess Mechanical Properties of Super- and Cyclic Contraction in Response to Environmental Humidity. SHAN LU, GANESH SWAMINATHAN, SAMUEL EVANS, TODD BLACKLEDGE, University of Akron — Major Ampullate (MA) spider silk is among the most impressive biomaterials due to its unparalleled mechanical properties, such as super-contraction and cyclic response to changes in humidity. Electropinning enables the generation of engineered silk fibers with controlled parameters and dimensions for various medical and commercial applications. However, their applications hinge on the ability to reproduce the mechanical properties such as a precise expansion-contraction response existed in natural silk fibers. Here, we successfully reproduced MA spider-silk fibers from solutions of natural MA silk proteins via electropinning, which exhibit the super-contraction and cyclic response to humidity change in a manner mirroring the natural fibers.

M1.00059 Investigation of ultrafast relaxation in terrestrial and meteoric Fe-Ni. LAURA CHEN, DANIEL EAKINS, DAVID CHAPMAN, SAM STAFFORD, JOHN WINTERS, Imperial College London, DAMIAN SWIFT, BASSEM EL-DASHIER, MIKE SACULLA, MUKUL KUMAR, JOEL BERNIER, Lawrence Livermore National Laboratory — The ablation and breakup of meteorites upon entry into the Earth’s atmosphere is an important challenge of global relevance. However, large thermal gradients, coupled with complex stoichiometry of Fe-Ni based meteorites, lead to difficulties in accurately modeling the breakup process. Ultrafast compression experiments are being conducted to better understand the effect of microstructure and temperature on the behavior of dislocation mechanisms in Fe-rich materials. The Janus laser at the Jupiter Laser Facility (LLNL) has been employed to drive pressures up to 50 GPa into thin foil targets composed of Fe and 0-25% atomic composition of Ni. Targets have been prepared from meteorites harvested from Diablo Canyon and the Gibeon crater, as well as Fe-Ni synthesized to yield similar stoichiometry. A new target holder has been used to pre-heat/cold targets in the range of 77-600K. Line-imaging VISAR and X-ray diffraction are employed to provide measure of distinct features linked to the onset of stress relaxation as well as to examine the effects of impurities on the \(\alpha\) - \(\epsilon\) phase transformation. In this poster, we present preliminary data of the effect of temperature and impurity content on the peak elastic state of Fe-Ni alloys under laser-driven shock compression.
M1.00060 Shock Thermodynamics of Mantle Rocks: Rockport Fayalite, SARAH STEWART, WILLIAM STEINHARDT, Harvard University — In order to address questions related to giant impacts and impact cratering on terrestrial planets, we need robust equations of state (EOS) and thermodynamic data for major mantle minerals (e.g., the olivine series and enstatite) and rocks under a wide range of pressure-temperature conditions. It is important to accurately characterize the amount of impact-induced heating that occurs in order to understand a range of planetary problems, including the mechanics of basin formation, the formation of the Martian crustal dichotomy, the origin of Earth’s moon, and the depths of magma oceans on the early Earth during accretion. The long-term goal of this work is to develop comprehensive EOS for the most important mantle minerals for use in impact modeling and to understand the heterogeneous distribution of shock and post-shock temperatures in rocks. Here we present the results from new post-shock temperature experiments on fine-grained Rockport fayalite rock and comparisons to previous post-shock measurements on rocks and minerals. Multi-band pyrometry data indicate that the post-shock temperature field is very heterogeneous in Rockport fayalite. We observe multi-wave shock profiles with VISAR in the mixed-phase region on the Hugoniot, which have not been previously recognized.

M1.00061 High Pressure Synchrotron X-ray diffraction and Raman Scattering Studies of Ammonium Azide, HONGYANG ZHU, XIAOXIN WU, HANG CUI, JIAN ZHANG, RIDONG CONG, QILIANG CUI, Jilin University — High-pressure in situ X-ray powder diffraction and Raman scattering studies on NH₄N₃ have been conducted up to 50.5 GPa and 48 GPa, respectively. The compressibility of orthorhombic ammonium azide is isotropic due to the orientation of azide anions. A given hydrogen bonding, taken with increasing pressure results in the increase of N−H−N bonding, leading to the increase of N−H stretch frequency and rotation of azide anions at 2b and 4h Wyckoff positions up to 2.9 GPa. The rotation of azide anions obviously influences the intermolecular interactions along c axis in orthorhombic phase. The pressure induced phase transition involves a proximity of α and c, temporarily assigned as a reversible second-order orthorhombic-to-tetragonal transition. The bulk modulus of the orthorhombic phases are determined to be K_{OT} = 24.5±3.5 GPa with K_{PT} = 3.4±3.2.

M1.00062 A view on the functioning mechanism of EBW detonation - Part 1: Electrical Characterisation, ELIZABETH LEE, RODNEY DRAKE, JOHN RICHARDSON, AWE Plc — This paper is the first of three characterising the initiation of PETN in an exploding bridgewire detonator to understand the underlying mechanism. The approach taken was to understand the transfer of energy through the system, beginning with the fireset / bridgewire interactions. The measurement of current, time to bridgewire burst and the transient voltage across the bridgewire at burst have enabled the determination of the energy used in bursting the bridgewire. This in turn has lead to the calculation of the energy efficiency of the fireset bridgewire system and an estimate of the energy delivered post bridgewire burst. It was postulated that this post-burst energy was responsible for the decrease in detonator function time as the firing energy is increased from threshold to all-fire levels. A fireset was designed to allow the post burst energy to be diverted away from the detonator, thus permitting the effect of the post burst energy on detonator function time to be quantified. The results of the experimental work will be presented, together with the implications for the initiation mechanism of PETN in an exploding bridgewire detonator.

M1.00063 Shock Initiation Thresholds of Various Energetic Materials, DAVID DAMM, Sandia National Labs, ERIC WELLE, Air Force Research Lab, COLE YARRINGTON, Sandia National Labs — Shock initiation threshold data for several energetic materials has been analyzed for both short-pulses and long, sustained shocks. In the limit of long duration shocks, the critical pressure for initiation is governed by the balance between chemical energy release in the vicinity of hotspots and thermal dissipation which cools the hotspot and can quench reactions. The observed trends in critical pressure from one material to the next are related to the thermophysical properties and chemical reaction kinetics of each material. Scaling analysis, combined with hydrocode simulations of collapsing pores has confirmed these trends; however large uncertainty in the reaction kinetics under shock loading prevents an accurate quantitative evaluation of the effects of specific planetary conditions.

M1.00064 X-ray diffraction studies of Mg$_2$Si and Ag-doped Mg$_2$Si under pressure, YOSHIHISA MORI, YUJI KAIHARA, KEN-ICHI TAKARABE, Okayama University of Science — The magnesium disilicide (Mg$_2$Si) is one of the thermoelectric material in 500-800 K temperature rage. The p- and n-Mg$_2$Si materials are necessary for the high-performance thermoelectric device, however Mg$_2$Si is n-type semiconductor and stable p-type Mg$_2$Si has not developed. Because it was reported that Ag-dope Mg$_2$Si was p-type Mg$_2$Si, we performed the X-ray diffraction studies of Mg$_2$Si and Ag-doped Mg$_2$Si under high-pressure at NE-5C beam line (PF-AR). Four samples which were a high-purity Mg$_2$Si powder, a mixture of Mg and Si powders, and Ag-doped these powders were powdered. Mg$_2$Si decomposed with increasing temperature, and new peaks of MgO and SiO$_2$ appeared beyond 673 K. The Mg$_2$Si with Ag also decomposed and the oxide peaks appeared, and Ag peaks did not disappear. In the case of Mg$_2$Si powder, Mg$_2$Si was synthesized at 573 K and Mg peaks disappeared with increasing temperature but MgO or SiO$_2$ peaks did not appear. In the case of Ag-doped Mg$_2$Si powder, Mg$_2$Si was synthesized at 523 K, and Ag peaks disappeared at 823 K and MgO or SiO$_2$ peaks did not also appeared. The result means the possibility of the synthesis of Ag-doped Mg$_2$Si under pressure.

1This work was supported by MEXT KAKENHI(C) Grant Number 11013342, and has been performed under the approval of the Photon Factory Program Advisory Committee (Proposal No. 2010G608, 2012G566).

M1.00065 Model-Based Development of a Small-Scale Experiment for Non-Shock Ignition of High Explosives, BRADLEY W. WHITE, H.K. SPRINGER, J.E. REAUGH, Lawrence Livermore National Laboratory, Livermore, CA 94555 USA — We demonstrate a model-based approach for developing small-scale experiments for non-shock ignition of high explosives (HEs) that are representative of abnormal environmental conditions. While small-scale experiments are often favored over large-scale testing since costs are lower and samples sizes are amenable to early stage HE formulation, concerns remain about the ability to predict full-scale non-shock ignition response. Our approach is to perform simulations of full-scale systems (i.e., Skid test) to identify the localized material extrema states (e.g., pressure, pressure duration, shear stress, strain-rate) underlying the non-shock ignition mechanism. The extrema states then provide a metric for iterative model-based development of small-scale experiments using a drophammer system. We performed these simulations using the HERMES (High Explosive Response to Mechanical Stimuli) model in the multiphysics code, ALE3D. Optimized experimental geometries reach 10s MPa pressures over 1-3 ms durations while inducing a large degree of shear. The results of the experimental development and the effects of design variations on non-shock initiation response of Comp B will be presented.

1This work performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344. This work was funded in part by the Joint DoD-DOE Munitions Program.
M1.00066 Equation of State for Detonation Product Gases, KUNIHITO NAGAYAMA, Kyushu University, SHIRO KUBOTA, National Institute of Advanced Industrial Science and Technology — Based on the empirical linear relationship between detonation velocity and loading density, an approximate description for the Chapman-Jouguet state for detonation product gases of solid phase high explosives has been developed. Provided that the Grüneisen parameter is a function only of volume, systematic and closed system of equations for the Grüneisen parameter and CJ volume have been formulated. These equations were obtained by combining this approximation with the Jones-Stanyukovich-Manson relation together with JWL isentrope for detonation of crystal density PETN. A thermodynamic identity between the Grüneisen parameter and another non-dimensional material parameter introduced by Wu and Jing can be used to derive the enthalpy-pressure-volume equation of state for detonation gases. This Wu-Jing parameter is found to be the ratio of the Grüneisen parameter and the adiabatic index. Behavior of this parameter as a function of pressure was calculated and revealed that their change with pressure is very gradual. By using this equation of state, several isentropes down from the Chapman-Jouguet states reached by four different lower initial density PETN have been calculated and compared with available cylinder expansion tests.

M1.00067 Effect of the oxygen balance on ignition and detonation properties of liquid explosive mixtures, MARC GENETIER, ANTOINE OSMONT, GERARD BAUDIN, CEA, DAM, Gramat — The objective is to compare ignition and detonation properties of various liquid high explosives having negative up to positive oxygen balance (OB): nitromethane (OB < 0), saccharose and hydrogen peroxide based mixture (quasi OB 0), hydrogen peroxide with more than 90% per wt (% w/o). The decomposition kinetic rates and the equations of state (EoS) of the liquid mixtures and detonation products (DP) are the input data for a detonation model. EOS are theoretically determined using the Woolfok et al universal liquid polar shock law and thermochemical computations for DP. The decomposition kinetic rate laws are determined to reproduce the shock to detonation transition for the mixtures submitted to planar plate impacts. Such a model is not sufficient to compute open field explosions. The aerial overpressure is well reproduced in the first microseconds, however, after it becomes worse at large expansion of the fireball and the impulse is underestimated. The problem of the DP EOS alone is that it takes into account only the detonation, the secondary combustion DP air being not considered. To solve this problem a secondary combustion model has been developed to take into account the OB effect. The detonation model has been validated on planar plate impact experiments. The secondary combustion parameters were deduced from thermochemical computations. The whole model has been used to predict the effects of the oxygen balance on open air blast effects of spherical charges.

M1.00068 The Deflagration of Energetic Crystals at Pressures above the Weak Shock Limit, STEPHEN GOVEAS, NEIL BOURNE, JEREMY MILLETT, AWE Plc — The response of inert solid to shock loading may be divided into two regimes of contrasting behaviour. In the lower of these, the material deforms in a regime below the theoretical strength of the material where deformation is triggered at discrete flaws. However, at pressures at grain boundaries, or second-phase particles, or vacancies within the lattice at the higher pressures, there comes a point, however, where the theoretical strength of the material is overcome and response becomes truly homogeneous behind the shock front and this point corresponds to the limit of weak shock behaviour within the crystal. Recent work of Zaug discussing burning rate of HMX as a function of pressure is reviewed and the onset of rapid deflagration is shown to commence as the WSL is exceeded. Implications for the shock response of energetic materials are discussed.

M1.00069 Shock initiation sensitivity and Hugoniot-based equation of state of Composition-B obtained using In situ electromagnetic gauging, L. LEE GIBSON, DANA DATTELBAUM, BRIAN BARTRAM, STEPHEN SHEFFIELD, RICHARD GUSTAVSEN, Los Alamos National Laboratory, CAROLINE HANDLEY, Atomic Weapons Establishment, SHOCK AND DETONATION PHYSICS TEAM, EXPLOSIVES MODELLING TEAM — Composition-B (Comp-B) is a solid cast explosive comprised of 59.5 wt % cyclotrimethylene-trinitramine (RDX), 39.5 wt% 2,4,6-trinitrotoluene (TNT), and 1 wt% wax. Its initial density depends on formulation method and as a result, the detonation properties of Comp-B have generally been studied at densities of 1.69 g/cm$^3$. The shock initiation sensitivity (Pop-plot) of Comp-B has been reported previously; obtained using both explosively-driven wedge tests and embedded manganese gauge techniques. We describe the results of a series of gas-gun-driven plate-impact initiation experiments on Comp-B ($\mu_0=1.72$ g/cm$^3$) using embedded electromagnetic gauges to obtain in situ particle velocity wave profiles at 10 Lagrangian positions in each experiment. From the wave profiles, an unreacted Hugoniot locus, the run-distance-to-detonation, and initiation waveforms are obtained in each experiment. The results indicate that Comp-B at $\mu_0=1.72$ g/cm$^3$ is more sensitive than reported previously. Comparisons are made of the new Hugoniot states with an earlier Hugoniot-based EOS. Measurements of the detonation wave profile using photonic Doppler velocimetry are also presented and discussed in the context of ZND detonation theory.

M1.00070 Pressure-Induced Irreversible Phase Transition in the Energetic Material Urea Nitrate, SHOURUI LI, BO ZOU, State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China — The behavior of energetic material Urea Nitrate (\textit{NH}_2\textit{C}_3\textit{OH} \cdot \textit{NO}_3 \cdot \textit{UN}) has been investigated up to the pressure of \textasciitilde 26 GPa. UN exhibits the typical supramolecular structure with uronium cation and nitrate anion held together by multiple hydrogen bonds in the layer. Both Raman and XRD data provide obvious evidence for the distorted phase transition in the pressure range \textasciitilde 9–15 GPa. Further analysis indicates phase II has Pc symmetry. The mechanism for the phase transition involves collapse of the initial 2D supramolecular structure to 3D hydrogen-bonded networks in phase Pc. Importantly, the transition is irreversible and leads to a large reduction in volume on release of pressure. The density in phase Pc has been increased by \textasciitilde 11.8% compared to the phase P2_1/c under ambient conditions and therefore phase Pc is expected to have much higher detonation pressure. This study opens new opportunities for preparing energetic materials with high density combining supramolecular chemistry with high-pressure techniques. Corresponding author. E-mail: zoubo@jlu.edu.cn Reference: JPC. 2013, 117, 152.

\textsuperscript{1} This work is supported by National Science Foundation of China (NSFC) (Nos. 91227202, and 21073071).

M1.00071 Comparison of Internal- Blast Explosive Performance in Small- and Large-Scale Tests, RICHARD GRANHOLM, NSWC Indian Head Division — Small-scale internal blast measurements were correlated with large-scale test data. Highly confined small explosive samples \textless 0.5 g were subjected to the output from a PETN detonator while enclosed in a 3-liter chamber. Large-scale tests up to 22.7 kg were generally unchanged and confined in a 180-m$^3$ chamber. When sample mass was expressed as total sample energy/chamber volume, theoretical peak quasi-static blast pressures for both small and large-scale tests fell on the same curve. Blast explosives may comprise high levels of fuels and reactive materials to enhance or control the release of energy, and may be insensitive and slow-reacting, with performance that may not scale well to small size tests. High confinement of a small sample can compensate for low sensitivity, but at the expense of heat loss to the metal confinement. This heat loss can be measured to improve the correlation between large and small-scale measurements, unless the released energy becomes too low to sustain complete reaction of the sample, either with itself or with air in the chamber.
M1.00072 Features of the Valorization of Single and Double Based Powders for Codetonation in Emulsion Explosives. JOSE B. RIBEIRO, RICARDO MENDES, BRUNO TAVERA, ADAI/LEDAP - Mechanical Engineering Department of the University of Coimbra, CRISTINA LOURO, CEMUC - Mechanical Engineering Department of the University of Coimbra — In this work, features of the thermal and detonation behavior of compositions resulting from the mixture of single and double based gun powder within ammonium nitrate (AN) based emulsion explosives are shown. That includes results of thermodynamic-equilibrium calculations of the detonation velocity, the chemical compatibility assessment through differential scanning calorimetry [DSC] and thermo gravimetric analysis [TGA], the experimental determination of the detonation velocity and a comparative evaluation of the shock sensitivity using a modified version of the "gap-test". DSC/TGA results for the compositions and for the individual components overlap until the beginning of the thermal decomposition which is an indication of the absence of formation of any new chemical specimens and so of the capability of the composition components. After the beginning of the thermal decomposition it can be seen that the rate of mass loss is much higher for the compositions with gun powder than for the sole emulsion explosive. Both, theoretical and experimental, values of the detonation velocity have shown to be higher for the powdered compositions than for the pure emulsion explosive. Shock sensitivity assessment have ended-up with a slightly bigger sensitivity for the compositions with double based gun powder when compared to the single based compositions or to the pure emulsion.

M1.00073 The Shock Response of Space Bears: The Ability of Life to Survive Some of the Most Extreme Environments Known to Man. JONATHON PAINTER, JAMES LEIGHS, GARETH APPLEBY-THOMAS, Cranfield University, RACHAEL HAZAEL, PAUL MCMILLAN, University College London, REINHARDT KRISTENSEN, University of Copenhagen — There have been many recent discoveries of life forms living in environments previously thought to be completely uninhabitable. One particularly interesting discovery of nature is the space bear or tardigrade. The name space bear is a colloquialism applied to the tardigrades because of a recent investigation which saw them being exposed to the vacuum of space and intense solar radiation, and surviving. Tardigrades have the ability to dehydrate themselves, entering a state called cryptobiosis. This state enables them to survive in the vacuum of space. A single stage gas gun has been employed to uniaxially shock load and subsequently recover tardigrades in both regular and cryptobiotic states. Loading histories were calculated via hydrocode modelling. Survival data is presented comparing shocked and control samples for tardigrades both in normal and cryptobiotic states.

M1.00074 Mechanical response of porcine skin under compression from low to high strain rates¹, CHIARA BO, Institute of Shock Physics, Imperial College London, BEN J. BUTLER, SMF Group, Cavendish Laboratory, Department of Physics, University of Cambridge, ALUN WILLIAMS, Department of Veterinary Medicine, University of Cambridge, KATHERINE A. BROWN, SMF Group, Cavendish Laboratory, Department of Physics, University of Cambridge, WILLIAM G. PROUD, Institute of Shock Physics, Imperial College London — Uniaxial compression experiments were performed on fresh porcine skin samples at different strain rates to study the stress-strain response. Low strain rate experiments were performed with an Instron 5566, while high strain rates were achieved using a Split Hopkinson Pressure Bar system. Magnesium bars and semiconductor strain gauges were used respectively to maximize the signal transmission from porcine skin to the output bar and to allow the signal measurement. Skin samples were harvested from different area of the animal to investigate the heterogeneity of such material. The experimental results showed that the mechanical response of skin in compression is strongly dependent on the strain rate of loading and on the location from which the samples were collected. Specimens collected from the rump showed a stiffer response compared to samples harvested from the thigh. Finally, a histological analysis of the samples post compression was carried out to examine the extent of tissue damage as a function of strain rate.

¹ This work is supported by the Atomic Weapons Establishment, UK and The Royal British Legion Centre for Blast Injury Studies at Imperial College London, UK.

M1.00075 Cylindrical shock waves and dynamic phenomena induced in solids by intense proton beams¹, ALESSANDRO BERTARELLI, FEDERICO CARRA, ALESSANDRO DALLOCCHIO, MICHAEL GUINCHARD, NICOLA MARIANI, LORENZO PERONI, STEFANO REDAELLI, MARTINA SCAPIN, None — The accidental impact of hadron beams on matter can induce intense shockwaves along with complex dynamic phenomena (phase transitions, extended density changes, explosions and fragment projections). These events have been successfully modeled resorting to wave propagation codes; to produce accurate results, however, these programs require reliable material constitutive models that are often scarce and inaccurate. A complex and innovative experiment was carried out at CERN to benchmark existing material constitutive models and possibly derive new ones. The test was based on the characterization of different materials impacted by intense proton beams and cylindrical shockwaves on material specimens and to observe the effects induced by their propagation. This method, a combination between numerical simulations and an experimental technique, permitting to tune the intensity, location and timing of the beam-deposited energy, may allow to study the effects induced by internal, quasi-instantaneous loadings in domains well beyond particle physics (accidents in nuclear facilities, internal explosions, high pressure blasts etc.), particularly when relatively little explored cylindrical shockwaves are generated.

¹ The research leading to these results has received funding from the European Commission under the FP7 Research Infrastructures project EuCARD, grant agreement no. 227579.

M1.00076 Strength and Sintering Effects at Ejection of Explosively Driven Sand. A.D. RESNYANSKY, S.A. WECKERT, Weapons Systems Division, DSTO, Edinburgh SA 5111, Australia — A description of sand response to extreme loads is very important for the evaluation of the sand ejecta effects to civilian and military targets. Sand is a complex material to simulate because of its porosity. With porous materials it is very hard to achieve the inter-phase equilibrium in shock waves. A previously developed two-phase model with strength has been implemented in CTH and applied to quartz sand. It has been shown that the Hugoniot abnormality known from the literature for highly porous silica is adequately described with the material non-equilibrium approach. Several models available in CTH may describe the flash X-ray observations available in the literature for the sand ejecta due to explosion of buried charges. However, a test-calculation divergence is noticeable when considering different burial depths. This is attributed to the material property variations due to the thermal sintering effects of the sand particles. Dynamic flash X-ray observations of aluminium plates loaded by ejected sand have been conducted, which has confirmed the material property variations in the ejected material. CTH calculations with a sintering kinetic implemented in the two-phase model improve description of the present tests and the sand ejecta tests at different burial depths.

M1.00077 Impact on porous targets: penetration, crater formation, target compaction and ejection³, EDUARDO BRINGA, CONICET and Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, 5500 Argentina, CHRISTIAN RINGL, HERBERT URBASSEK, Fachbereich Physik und Forschungszentrum OPTIMAS, Universität Kaiserslautern, Erwin-Schroedinger-Straße, D-67663 Kaiserslautern, Germany — Using a granular-mechanics code, we study the impact of a sphere into a porous adhesive granular target, consisting of monodisperse silica grains. The model includes elastic repulsive, adhesive and dissipative forces, as well as sliding, rolling and twisting friction. Impact velocities up to 30 m/s, and target filling factors (densities) between 19% and 35% have been systematically studied. We find that the projectile is stopped by an effective drag force which is proportional to the square of its velocity. Target adhesion influences projectile stopping only below a critical velocity, which increases with adhesion. The penetration depth depends approximately logarithmically on the impact velocity, and is inversely proportional to the target density. The excavated crater is of conical form and is surrounded by a compaction zone, whose width increases, but whose maximum value decreases with increasing target density. Grain ejection has been conducted, which has confirmed the material property variations in the ejected material. CTH calculations with a sintering kinetic implemented in the two-phase model have shown to be quite effective for predicting the target filling factors (densities) between 19% and 35% have been systematically studied. We find that the projectile is stopped by an effective drag force which is proportional to the square of its velocity. Target adhesion influences projectile stopping only below a critical velocity, which increases with adhesion. The penetration depth depends approximately logarithmically on the impact velocity, and is inversely proportional to the target density. The excavated crater is of conical form and is surrounded by a compaction zone, whose width increases, but whose maximum value decreases with increasing target density. Grain ejection increases in proportion with impactor velocity and the angular distribution of the ejecta has a maximum around 45 degrees respect to the surface normal.

³ This work has been supported by the Deutsche Forschungsgemeinschaft via the Graduiertenkolleg 814. E.M.B. acknowledges support from CONICET, SeCTyP (U.N. Cuyo), and PICT-2009-0092.
M1.00078 An overview on the effect of manufacturing on the shock response of polymers. GUILLAUME KISTER, DAVID WOOD, GARETH APPLEBY-THOMAS, ANDREW ROBERTS, JAMES LEIGHTS, MICHAEL GOFF, AMER HAMEED, Cranfield University — Polymers are widely employed in areas as diverse as consumer goods and explosives (matrix materials). The consequent commercial interest has led to a continual drive to improve material properties — e.g. via either manufacturing techniques or more fundamental improvements in the understanding of the underlying chemistry. It has been shown previously that chemical compositions can affect the shock profile of the polymer Poly-Methyl Methacrylate (PMMA). To this end the composition will change over time as new formulations are brought to market, for example due to the inclusion of additives that will influence the life time of the polymer. The challenge of significantly such changes may not affect the material properties at lower strain rates. At the higher strain rates these subtle differences can lead to larger discrepancies in the shock profiles. In this study comparisons of PMMA have been made between newly sourced and “legacy” material studied previously in the literature.

M1.00079 Experimental study on shear failure of polypropylene under shock loading1, ZHIPING TANG, TING LI, Univ. of Sci. and Tech. of China — The impact response of crystallized polypropylene under combined compression and shear loading was studied by using the inclined gas gun and the IMPS system. The experimental results show that the transverse wave velocity increases nonlinearly with the impact velocity. Therefore, the shear stress wave velocity is strongly related to the hydrostatic pressure. Penetration shear wave attenuation occurs near the impact surface when the impact velocity and inclination angle reach the critical value. The micro-observation of recovered samples with a polarized optical microscope reveals that there exists a melting layer of about 2-3 µm thick, i.e. adiabatic shear failure layer, very near the impact surface (about 5µm) which causes the shear wave attenuation.

1Supported by the Chinese National Natural Science Foundation (11272311)

M1.00080 Shocks Properties of Anisotropic Polymers, GARETH TEAR, DANIEL EAKINS, DAVID CHAPMAN, WILLIAM PROUD, Institute of Shock Physics, Imperial College London — The effect of anisotropy in polymer materials caused by the alignment of polymer chains during manufacture and processing has been previously investigated at low strain rates by multiple authors, however the effect of molecular orientation at higher strain rates and shock loading is an area of active research. This work presents experimental results on the effect of molecular orientation on shock propagation in polycarbonate. The Us – Uhgioniot has been measured for varying degrees of chain alignment. Polycarbonate is an amorphous polymer which does not exhibit cross-linking, allowing the study and modeling of the material to be simplified. Birefringence is used to study the initial anisotropy of the material before loading. During loading optical techniques are used to characterize shock behavior, namely line VISAR, Het-V/PDV and high-speed imaging. The influence of strain orientation has been studied, including the effect of high speed imaging in conjunction with birefringence as a method of qualitatively analyzing shock induced anisotropy in optically transparent polymers.

M1.00081 Rate Dependent Shear Failure and the Scaling Effect in Long Rod Penetration, YEHUDA PARTOM, Retired — Long rod penetration tests show a scaling effect that cannot be explained by rate dependent strength. We propose here that this scaling effect may be explained by rate dependent failure. We start by revisiting the well known result, that long rod penetration efficiency depends on the strain to failure of both projectile and target materials. We then make the strain to failure depend on strain rate, using the overstress concept. In this way the effective strain to failure increases with strain rate. As strain rate increases with decreasing scale, we get that penetration efficiency decreases with decreasing scale as observed in tests. In the paper we show results of hydrocode runs that demonstrate the relation between strain rate sensitivity of the strain to failure, and the scaling effect in long rod penetration.

M1.00082 Modeling Combined Tension-Shear Failure of Ductile Materials, YEHUDA PARTOM, Retired — Failure of ductile materials is usually expressed in terms of effective plastic strain. Ductile materials can fail by two different failure modes, shear failure and tensile failure. Under dynamic loading shear failure has to do with shear localization and formation of adiabatic shear bands. In these bands plastic strain rate is very high, dissipative heating is extensive, and shear strength is lost. Shear localization starts at a certain value of effective plastic strain, when thermal softening overcomes strain hardening. Shear failure is therefore represented in terms of effective plastic strain. On the other hand, tensile failure comes about by void growth under tension. For voids in a tension field there is a threshold state of the remote field for which voids grow spontaneously (cavitation), and the material there fails. Cavitation depends on the remote field stress components and on the flow stress. In this way failure in tension is related to shear strength and to failure in shear. Here we first evaluate the cavitation threshold for different remote field situations, using 2D numerical simulations with a hydrocode. We then use the results to compute examples of rate dependent tension-shear failure of a ductile material.

M1.00083 Evolution of shock compression waves in a SiC ceramic, ANDREY S. SAVINYKH, Institute of Problems of Chemical Physics of RAS, Chernogolovka, Russia, Gennady I. KANEL, Joint Institute for High Temperatures of RAS, Moscow, Russia, SERGEY V. RAZORENOV, Institute of Problems of Chemical Physics of RAS, Chernogolovka, Russia, VLADIMIR I. RUMYANtSEV, LLC VIR, Saint-Petersburg, Russia — The objective of this study was to estimate possible contribution of stress relaxation into the response of hard ceramic materials to high-rate compression and tension. With this goal, the free surface velocity histories have been measured for plane SiC ceramic samples of 0.07 g/cm³ density subjected to impact by a flyer plate. The sample thickness was varied from 0.5 mm up to 8.3 mm. The peak shock stress was in a range of 17.9 - 21.9 GPa. The Hugoniot elastic limit (HEL) is in a range of 8.34 to 8.72 GPa for this material, the spall strength value is 0.5 to 0.62 GPa. Both the HEL and the spall strength are in reasonable agreement with literature data for SiC ceramics of corresponding density. Measurements have not revealed any decay of the elastic precursor wave. Moreover, it has been found the evolution of the compression wave is practically self-similar and is well described by the simple wave approach. It follows from these observations the stress relaxation does not provide significant contribution into the response of hard ceramic materials to shock-wave loading. The ramped transition from elastic to plastic wave is caused by strain hardening of the material and by successive involving of grains of various orientations into the inelastic deformation process.

M1.00084 Numerical-theoretical analysis of destruction of liquid drop under effect of air shock wave, ALLA GEORIEVSKAYA, YVCTOR RAEVSKY, RFNC-VNIIEF — Direct numerical simulation of liquid fragmentation in gas flow is rather complicated. It is caused by the need for specifying a large number of points, and, therefore, use of superpower computers. On the other hand, surface tension is the characteristic, which determines drop sizes. It is very difficult to simulate this characteristic in calculations. When using the presently available techniques, numerical calculations reproduce some moments of interaction between liquid and air shock wave only at the qualitative level. However, these calculations allow obtaining the change of strain rate average in drop volume versus time, and finally estimating the average particle sizes. We performed similar calculations for drops with different initial diameters. It allowed estimating the influence of scale effect on average size of particles and their final distribution in sizes. Results of the numerical-theoretical investigations are compared to results of experiments, which were performed in VNIIEF.

M1.00085 Probabilistic Approach to Numerical Simulation of Fracture, ALEXANDER GERASIMOv, Tomsk State University — The natural heterogeneity of real materials structure influencing on distribution of material physico-mechanical characteristics (PMC) is one of the factors determining character of destruction. The introduction of the given factor in the equations of mechanics of a deformable solid is possible at use probabilistic laws of distribution PMC on volume of a considered design. There are problems where the fragmentation is mainly probabilistic process: explosive destruction axisymmetric shells where character of blasting fragmentation are beforehand unknown. Determining influence of heterogeneity of material structure is shown as well in problems punching thin barrier. In order that simulated process of a fragmentation reflected a real picture of behavior of the destroyed bodies, it is necessary to bring in casual distribution of initial deviations strength properties from rating value to PMC of a body. In work the explosive fragmentation of the shells, a fragmentation of a barrier and an shell after barrier piercing, punching thin barrier on a normal and under an angle, crushing of metal rings, process of high-speed impact of the laminated - spaced barrier with the steel spheres is considered.
M1.00086 Intragranular fracture and frictional effects in granular materials under pressure-shear loading. AMANDA PETERSON, JOHN FOSTER, The University of Texas at San Antonio, TRACY VOGLER, Sandia National Laboratories — Research efforts have been undertaken in recent years to investigate the dynamic behavior of granular materials. Many of the investigations have been experimental in nature, consisting of several rounds of Kolsky bar tests on sand with varying moisture content and confining pressures as well as traditional plate impact. More recently, pressure-shear experiments on both sand and granular tungsten carbide have been performed. In order to investigate the mesoscale physics that affect the bulk response observed in experiments, we have undertaken a computational simulation effort. The simulations are conducted using a massively parallel computational peridynamics code capable of modeling many grains at high resolution resulting in simulations that consist of several million degrees of freedom. Individual intragranular fracture and discrete contact with friction are modeled explicitly in the simulations. Thus, these simulations treat aspects of the problem that were not represented well in previous mesoscale simulations with Eulerian hydrocodes. Results from these simulations are compared with results from pressure-shear experiments on sand and granular tungsten carbide. A discussion of the effects of fracture and friction on force chain formation and bulk wave propagation in the samples is included.

M1.00087 Molecular Dynamics Modelling of Laser-Pulse Compression of a Ta single crystal with dislocations1, CARLOS J. RUESTES, ICB-UNCUYO & University of California, San Diego, La Jolla, CA 92039, USA, TANE P. REMINGTON, University of California, San Diego, La Jolla, CA 92039, USA, EDUARDO M. BRINGA, ICB-UNCUYO & CONICET, Mendoza 5500, Argentina, MARC A. MACHADO, University of California, San Diego, La Jolla, CA 92039, USA, BRUCE A. REMINGTON, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA — The nanoindentation of a defect-free Ta [001] single crystal is studied by Molecular Dynamics simulations. The potential by Li et al [PRB 67 (2003)], an EFS potential [J Phys Condens Matter 18(2006)], and a recent EAM potential by Ravelo et al [AIP Conf Proc 1426 (2012)] are tested and their results analyzed in terms of dislocation slip planes. Dislocations emitted from the indented zone interact forming prismatic loops. The Ta dislocated structure is then subjected to shock compression induced by a piston hitting the sample at various speeds. The shock-induced dislocation generation and motion mechanisms are studied in order to compare to on-going experiments.

1This research was funded by ANPCyT PRH, PICT2008-1325, PICT2009-0092, SecTyP UNCuyo 06/M035 and UC Research Lab grants

M1.00088 Dynamic Fracture of Borosilicate Glass with Plasma Confinement geometry in Pure Water by Laser-induced Shock Wave, FUMIKAZU SAITO, HIROAKI KISHIMURA, TAKANORI SUZUKI, National Defense Academy — In order to characterize dynamic fracture of borosilicate glass, we performed laser-shock-experiments of both an aluminum-ablator mounted glass and a glass with plasma confinement geometry in pure water by Q-switched Nd:YAG laser. The incident beam with 440 mJ was focused onto the target approximately 300 µm in diameter. The dynamic fracture of the glass targets is observed with high-speed digital framing-camera photography. For the aluminum-ablator mounted glass, propagation of the shock wave in water was observed, and the shock-wave velocity is obtained to be 1.65 ± 0.02 km/s using image processing. Shock-pressure applied the target is estimated to be 180 MPa by Hugoniot relation. For the glass with plasma confinement geometry, generation of the micro-fragments from the rear side of the target was observed. This result indicates that shock-induced fragmentation by laser irradiation is enhanced by the plasma confinement effect. The soft-recovered fragments are separated according the size with PET mesh having deferent mesh size. As a result, the glass with plasma confinement geometry generated smaller fragment than the aluminum-ablator mounted glass.

M1.00089 Study on the selectivity of damage nucleation at the boundaries of ductile metal, DUAN FAN, MEILAN QI, School of Science, Wuhan University of Technology — Voids nucleation is the first stage of fracture in ductile materials. The location and number of nucleation is the key to predict when and where the fracture will take place. Studies show that the nucleation mainly occurs at the grain boundaries in high-purity polycrystalline metals. However, the nucleation and growth does not occur uniformly. This project seeks to test the response of large-grain polycrystalline metal samples with different grain boundary structure under the same loading conditions and then recovers the samples. The resulting tensile damage in the recovered samples is examined by optical, electronic backscatter diffraction analysis of the technology (EBSD), and transmission electron microscopy (TEM). The distribution and mechanism of the nucleation will be studied at different grain boundaries, and a nucleation model will be established for finite element analysis, which can be used to predict the damage nucleation at complex grain boundary conditions (including textured polycrystalline). Finally, the result will be verified by experiment.

M1.00090 Spall and Damage Behavior of Intrinsically-Reinforced Bulk Metallic Glass Composites, RENE DIAZ, GREG KENNEDY, Georgia Institute of Technology, DOUGLAS HOFMANN, NASA Jet Propulsion Laboratory, NARESH THADHANI, Georgia Institute of Technology — We have performed uniaxial-strain plate-impact experiments to study the strength and spall damage of bulk metallic glass-matrix composites (BMGMCs). BMGMCs counteract the brittle nature of monolithic BMGs through in-situ formed crystalline dendrites which increases toughness and ductility. Applications for micrometeoroid shielding, kinetic energy penetrators (KEP) and armor shielding raises the question of the dynamic stability of BMGMCs. Microstructures of BMGMCs were investigated using uniaxial-strain plate-impact experiments to examine the phase stability of the dendrite-reinforced BMGMCs under high pressure and their high strain-rate deformation and failure response. The experiments involve impact of 303 stainless steel flyer plate on 303 stainless steel sample holder containing two BMGMC samples at varying velocities. The Hugoniot Elastic Limit (HEL) and the spall strength of the BMGMC samples was determined using velocity interferometer system for any reflector (VISAR). Post-mortem microstructural characterization is done on the recovered sample and correlated with the measured damage response. The results obtained will be dated to present.

M1.00091 Strength and destruction of flat amorphous during shock–wave tests, OLEG DRENNOV, ANATOLY MIKHAILOV, ALEKSEY FEDOROV, RFNC-VNIIEF — Devices with nondestructive plane ampoules which permit testing specimens with volume up to 35 cm3 under different conditions of explosive action with the intensity up to 100 GPa included are developed. Strength properties of ampoules made of different steels are evaluated under dynamic loading. These devices and ampoules are used for study of physical and chemical processes, which occur in substances under pulse effects of high strain rate, pressures and temperatures. The most promising materials are determined. Schemes are presented for flat recovery ampoule and loading devices required for providing the following loading conditions: 10 GPa ≤ P ≤ 100 GPa; 0.5 µs ≤ τ ≤ 5 µs. Peculiarities are described for application of the considered recovery ampoules:

- to test samples, which undergo volume reduction;
- to test fusible samples;
- to test samples when loading by oblique shock wave.

M1.00092 On the importance of the 7.62 mm FFV bullet jacket during penetration, ANDREW ROBERTS, Cranfield University, PAUL HAZELL, The University of New South Wales, GARETH APPLBY-THOMAS, AMR HAMEED, MICHAEL GIBSON, Cranfield University — While a critical part of the bullet structure, relatively little attention has traditionally been paid to the effects of the jacket during penetration. Recent work has suggested that the jacket of a 7.62 mm FFV projectile measurably affects penetration into ceramic-faced targets. In this study a series of both forwards and reverse ballistics shots employing 7.62 mm FFV rounds accelerated into c.a. 830 m/s (and vice-versa) were undertaken. The various FFV rounds were prepared with differing degrees of jacket modification about their tip. Penetration mechanisms were interrogated using a multi-channel flash X-ray system, while a series of depth-of-penetration tests provided a route to quantitatively assess the contribution of the jacket to penetration.
M1.00093 A study of the elastic precursor in thin Zr and Ta foils, DANIEL EAKINS, DAVID CHAPMAN, Imperial College London — The evolution of the elastic precursor with strain rate and distance contains rich information regarding the origins of yielding under intense dynamic loading. Such information is necessary for the development of new dislocation-based strength models. In this work we extend study of elastic precursor behavior in zirconium and tantalum foils down to 25 \( \mu \text{m} \) to address the role of reduced thickness and crystal symmetry on the kinetics of stress relaxation. Using a newly constructed mesoscale gas launcher, high purity Zr and Ta targets ranging in thickness from 6 nm down to 25 \( \mu \text{m} \) have been impacted at velocities of \( \sim 500 \text{ m/s} \). A combination of line-imaging VISAR and frequency-shifted PDV was employed to measure the particle velocity at a windowed interface. Features of the elastic precursor in the breakout profiles, such as the peak elastic state and yield drop, were used to infer the kinetics of incipient relaxation processes. In future work, these results will be used to further validate the D3P code currently under development.

M1.00094 Monte Carlo calculations of liquid metals surface tension, EMEC BOURRASSEAU, AHMED-AMINE HOMMAN, OLIVIER DURAND, CEA — Large scale molecular dynamics (MD) simulations have been performed in our group to study and to model the ejection production from the dynamic fragmentation of shock-loaded metals under melt conditions. Those microscopic simulations show that the modeling of such phenomena using hydrodynamic codes will imply the understanding of the physics occurring at the surface of the liquid fragments. Thus, it appears that surface tension will be one of the overriding properties to be taken into account in the hydrodynamic codes. As a consequence, we report here Monte Carlo calculations of surface tension of liquid metals using both mechanical and thermodynamic approaches.

M1.00095 Atomistic Mechanism of Plastic Deformation During Nano-indentation of Titanium Aluminide, JOSE PEDRO RINO, Universidade Federal de Sao Carlos, CLAUDIO J. DASILVA, Pontifícia Universidade Católica de Goiás — The mechanisms governing defect nucleation in solids are of great interest in all material science branches. Atomistic computer simulations such as Molecular Dynamics (MD), have been providing more understanding of subsurface deformations, bringing out details of atomic structures and dynamics of defects within the material. In the present work we show the first simulation measurements within an atomistic resolution of the mechanical properties of titanium aluminide intermetallic compound (TiAl), which is a promising candidate for high temperature applications with remarkable properties, such as: attractive combination of low density, high melting temperature, high elastic modulus, and strength retention at elevated temperatures, besides its good creep properties. Through calculations of local pressure, local shear stress and spatial rearrangements of atoms beneath the indenter, it was possible to quantify the indentation damage on the structure. We have founded that prismatic dislocations mediate the emission and interaction of dislocations and the activated slip planes are associated with the Thompson tetrahedron. Furthermore, using the load-penetration depth response, we were able to estimate the elastic modulus and the hardness of the TiAl alloy. All our findings are in well agreement with experimental results.

M1.00096 ABSTRACT WITHDRAWN

M1.00097 Theoretical determination of anisotropic thermal conductivity for crystalline 1,3,5-triamino-2,4,6-trinitrobenzene (TATB)\(^1\), MATTTHIE P. KROONBLAWD, THOMAS D. SEWELL, Department of Chemistry, University of Missouri-Columbia — Bond stretching and three-center angle bending potentials have been developed to extend an existing rigid-bond TATB molecular dynamics (MD) force field (FF) for simulations requiring fully flexible molecules. The FF potentials were fit to experimental vibrational spectra and electronic structure predictions of vibrational normal modes and frequencies using a combination of zero Kelvin eigenmode analysis for the isolated molecule and finite-temperature power spectra for the isolated molecule and bulk crystal. Crystal structures computed using the revised FF are in good agreement with results from other computational models and experimental data. A non-equilibrium MD method was used to obtain the room temperature, atmospheric pressure thermal conductivity along three directions in a well-defined, non-orthogonal basis. The thermal conductivity was found to be significantly anisotropic with values of \(1.13 \pm 0.07, 1.07 \pm 0.07 \) and \(0.65 \pm 0.03\) W m\(^{-1}\) K\(^{-1}\) for directions nominally parallel to the \(a\), \(b\), and \(c\) crystal directions, respectively.

\(^1\)The U.S. Air Force Office of Scientific Research supported this research.

M1.00098 High pressure XAS and XMCD studies on the ODE beam line at SOLEIL , LUCIE NATAF, FRANCOIS BAUDELET, QINGYU KONG, SEBASTIEN CHAGNOT, Synchrotron SOLEIL — X-ray Absorption Spectroscopy (XAS) is a very useful probe to obtain local information in materials science. It is suitable for a variety of compounds, since a long-range order is not required. Matsushita has been the first to propose an alternative to the classical method of recording absorption spectra: the dispersive set-up. Instead of scanning the energy step by step, only one crystal is used and bent in such a way that it directly opens an energy range and focuses the beam. Since then, a few beam lines have been developed on this idea, the ODE beam line of the SOLEIL Synchrotron is one of them. Absorption measurements using this set-up present the advantages to be very fast (down to a few \(\mu\text{s}\)) and very stable, since no mechanical movements are required. These characteristics make the dispersive XAS technique suitable for investigating small samples, following kinetics and measuring small signal to noise ratio (down to \(10^{-5}\)). Thanks to its focusing optics, the dispersive set-up is very well adapted to high pressure, the sample chamber being typically of about \(100\mu\text{m}\) in diameter and \(20\mu\text{m}\) in thickness. Moreover, the ODE beam line is built on a bending magnet allowing a circular polarization of the beam, hence providing X-ray Magnetic Circular Dichroism (XMCD) measurements. In this poster, we will present some XMCD and fast kinetic results recently obtained and the last improvements of the ODE beam line.

M1.00099 Methods for processing experimental data in microwave diagnostics of shock waves and detonation, ALEXANDER SEDOV, ALEXEY RODIONOV, RFNC-VNIIEF, Sarov, VLADIMIR KANAKOV, Lobachevsky NNSU, Nizhny Novgorod — Microwave interferometry is a promising method of unperturbing diagnostics of short-time processes. It is a bit less effective than the optical methods in accuracy, but it provides a researcher with more capabilities, in particular, for measurements in optically opaque media. The classic methods for processing experimental interferograms using extremums allow to obtain data on motion of investigated objects with the resolution of a quarter of wavelength of probing radiation. It is insufficient for majority of practical applications. Use of the mathematical methods for processing output signals of the receiver allows to improve the method resolution significantly and to obtain motion measurement errors of 0.05...0.1 of wavelength or even less. This paper presents schemes of conduction and brief description of the methods for processing a series of tests, which were performed in RFNC-VNIIEF with use of radio interferometer having length of wave of probing radiation \(\lambda = 3.2\) mm, namely:

- to measure velocity of stationary detonation;
- to measure depth of detonation initiation by shock wave;
- to investigate shock compressibility of dielectric materials;
- to investigate dynamics of constructions.
M1.00100 Advanced target configurations for gigabar equation of state experiments at the National Ignition Facility

K.T. SULLIVAN, J. KUNTZ, D.C. SWIFT, J.A. HAWRELIAK, A. KRITCHER, T. DOEPPNER, Lawrence Livermore National Laboratory — The initial version of the converging-shock equation of state (EOS) platform demonstrated at NIF used a configuration based as closely as possible on inertial confinement fusion (ICF) targets. The success of this platform and the accuracy of the design simulations gives confidence that future experiments can be more flexible in both the hohlraum and target configurations. Changes in the target will enable significant improvements in EOS measurements. The first targets used a proven ICF ablator design, and the sample was a uniform sphere of CH-based plastic. As well as optimizing designs for other sample compositions, we are developing methods of fabricating samples with buried radiographic marker layers—a narrow layer with a high-Z dopant—using direct ink writing and electrophoretic deposition. The incorporation of multiple marker layers is an important step forward in converging shock experiments. The particle speed can be measured directly as the shock passes, and an average compression and opacity can be determined directly from the separation between markers and local x-ray attenuation. The markers can also be used to improve the precision of the radiographic unfold used to reconstruct the spatial dependence of the compression and opacity profiles. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

M1.00101 High-pressure and high-temperature mineral-fluid interface cell for high-resolution x-ray reflectivity measurement

CHANGYONG PARK, CURTIS KENNEY-BENSON, HPCAT, Geophysical Laboratory, Carnegie Institution of Washington — Ordering of water at the mineral-fluid interface is a fundamental process governing mineral hydration, ion-adsorption, dissolution, growth, and charge transfers across the mineral surface. However, the influence of pressure and temperature on this fundamental process is still largely unknown. The experimental determination is limited due to the lack of a sample cell which can properly handle the pressure and temperature of the fluidic component and simultaneously allow measurement of the interfacial structure, e.g., by high-resolution x-ray reflectivity. We recently developed a new high-pressure and high-temperature mineral-fluid interface cell to achieve the high-resolution x-ray reflectivity measurement from single crystalline mineral surfaces under the PT conditions of fluid up to ~750 K and ~40 MPa. The interfacial structures at single crystal mineral surfaces interacting with various hydrothermal fluids will promote our understanding of the molecular aspects of hydrous alteration processes of rocks in deep Earth environments. The application can be extended to mineral surface sciences, geological carbon sequestration, and nuclear engineering.

M1.00102 Explosive Welding of Pipes

OLEG DRENNOV, ANDREY DRENNOV, OLGA BURTSEVA, RFNC-VNIIEF — For connection by welding it is suggested to use the explosive welding method. This method is rather new. Nevertheless, it has become commonly used among the technological developments. This method can be advantageous (saving material and physical resources) comparing to its statical analogs (electron-beam welding, argon-arc welding, plasma welding, gas welding, etc.), in particular, in hard-to-reach areas due to their geographic and climatic conditions. Explosive welding of cylindrical surfaces is performed by launching of welded layer along longitudinal axis of construction. During this procedure, it is required to provide reliable resistance against radial convergent strains. The traditional method is application of fillers of pipe cavity, which are dense cylindrical objects having special designs. However, when connecting pipes consecutively in pipelines by explosive welding, removal of the fillers becomes difficult and sometimes impossible. The suggestion is to use water as filler. The principle of non-compressibility of liquid under quasi-dynamic loading is used. In one-dimensional gasdynamic and elastic-plastic calculations we determined non-deformed mass of gas (perturbations, which are moving in the axial direction with sound velocity, should not reach the layer end boundaries for 5-7 circulations of shock waves in the radial direction). Linear dimension of the water layer from the zone of pipe coupling along axis in each direction is ≥2R, where R is the internal radius of pipe.

M1.00103 Textile dry cleaning in high pressure CO2

STEVIA SUTANTO, TU Delft, MAAIKE VAN DER KAMP, Feyecon Carbon Dioxide Technologies, GEERT-JAN WITKAMP, TU Delft — High-pressure carbon dioxide (CO2) is one of the most suitable replacements for perchloroethylene (PER), a common but harmful textile dry cleaning solvent. Previous studies have indicated that the particulate soil removal with CO2 is lower compared to that with PER, because of the lesser amount of mechanical action in CO2. Furthermore, there is a lack of understanding of textile-dirt-CO2 interaction. It is the objective of this study to get an insight in the mechanical forces that play a role in CO2 dry cleaning and to use this information to improve the CO2 washing performance. Various mechanical actions were investigated with the experiments in an in-situ high pressure observation cell. Textiles stained with different kinds of particulate soils were washed in CO2. The washing results show that the combination of rotating and vertical action gives the highest cleaning performance and liquid CO2 spray may be a suitable additional mechanism to increase the cleaning performance.

M1.00104 Combined Laser Ultrasonics, Laser Heating and Raman Scattering in Diamond Anvil Cell System

PAVEL ZININ, University of Hawaii, VITALI PRAKAPENKA, University of Chicago, SHOKO ODAKE, KATHERINE BURGESS, University of Hawaii — We developed a unique and multifunctional in-situ measurement system under high pressure equipped with laser ultrasonics system (Raman device, and laser heating system (LU-LH-DAC) at the University of Hawaii. The system consists of four components: (1) LU-DAC system (probe and pump lasers, photodetector, and oscilloscope); (2) a fiber laser (1064 nm), which is designed to allow precise control of the total power in the range from 2 to 100W by changing the diode current, for heating samples; (3) a spectrometer for measuring the temperature of the sample (using Black body radiation), fluorescence spectrum (spectrum of the ruby for pressure measurement), and Raman scattering measurements inside DAC under high pressure and high temperature (HPHT) conditions; and (4) an optical system for focusing laser beams (pump, probe, and 100W CW lasers) on the sample in DAC and for imaging a sample inside the DAC. The system allows us to: (a) measure acoustical properties of materials under HPHT; (b) synthesize new phases under HPHT; and (c) measure Raman scattering under HPHT conditions for detection of phase transition.

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9:15AM O1.00002 The Role of Defect Kinetics on Spall Failure. JUSTIN WILKERSON, K.T. RAMESH, Johns Hopkins University — Spall failure is a complex multiscale, multirate process. During the shock compression, the material undergoes a myriad of shock stress magnitude and pulse duration dependent microscopic processes that may include dislocation multiplication, nucleation, trapping, pile-up, annihilation, recovery, cell evolution, as well as vacancy generation and clustering. In addition to shock hardening the material, this new shock induced defect structure seeds the material with new potential void nucleation sites that may be activated during the proceeding period of dynamic tensile loading. Upon nucleation, the voids undergone dynamic growth to coalescence, constrained by inertia and viscoplastic resistance to deformation. A predictive micromechanical model is developed to analyze the role of these time-dependent processes in the experimentally observed spall strength dependence on initial microstructure, preheat temperature, tensile loading rate, and shock stress magnitude. In addition, simple spall strength scaling laws that capture the essential physics and microstructure dependence will be presented.

10:00AM O1.00003 ABSTRACT WITHDRAWN

10:15AM O1.00004 Experimental investigation of shock-wave processes in solid and liquid paraffin. ALEXANDER UTKIN, VASILIY SOSIKOV, IPCP RAS — Paraffin response to shock-wave stressing at transition through melting temperature have been researched. The homogenized paraffin and docosane (C_{26}H_{62}) were investigated at initial temperature of 20 and 70 °C. Compression pulse amplitude was changed from 0.2 to 2 GPa. Registration of free surface velocity was made with VISAR laser interferometer. It was shown that phase transition of paraffin from solid to liquid state does not lead to appearance of any features on wave profiles. Spall strength remains constant an it equals to about 25 MPa independent to state of sample. Significantly different results were achieved in experiments with docosane. In liquid phase velocity profiles are similar to paraffin but the spall strength is higher and equals to 40 MPa. In solid state the spall strength halves, and dramatic change of compression pulse structure is observed. If in liquid phase shock jump forms, then in solid state two wave configuration is recorded. Moreover the front of compression pulse expands during propagation. It means that solid docosane has an elastic property which leads to formation of forerunner and its compressibility is anomalous at low pressures.

10:30AM O1.00005 Study on Dynamic Fragmentation of Multiple Metal Rings under High Explosive Loading. TIEGANG TANG, GUOWU REN, ZHAOLIANG GUO, QINGZHONG LI, Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang 621900 — An experimental platform for metal expanding ring incorporating with exploding wire technique is set up to improve the instability of high explosive loading. The experimental designs including the circuit control and test performance are illustrated in great detail. Furthermore, on the basis of this technique we investigate dynamic fragmentation of multiple rings stacked on a metal driver. The statistical distribution of recovered fragments is discussed.


9:15AM O2.00001 Density Functional Theory simulations of shock compression of porous tantalum pentoxide\textsuperscript{1}. K. COCHRANE, T.J. VOGLER, S. ROOT, M.P. DESJARLAIS, L. SHULENBURGER, T.R. MATTSSON, Sandia National Laboratories — Density Functional Theory (DFT) based molecular dynamics has been established as a method capable of yielding high fidelity results for many materials at a wide range of pressures and temperatures and has recently been applied to complex polymers such as polyethylene, compounds such as ethane or CO\textsubscript{2}, and oxides such as MgO. We use this method and a modification to the Rankine-Hugoniot relation inspired by the P\textsubscript{crush} model to extend the DFT approach to the calculation of the shock response of an initially porous tantalum pentoxide. The experimental data have initial densities of approximately 1 g/cc, 3 g/cc, and 7 g/cc, reduced from a normal density of 8.36 g/cc, with final pressures up to 200 GPa. The DFT results compare well with the 3 g/cc and 7 g/cc over a wide range of pressures. The agreement with the 1 g/cc Hugoniot experimental data is reasonable at lower pressures, but with some larger discrepancies at higher pressures. Finally, we calculate the Gruneisen gamma as a function of density and found that it is density dependent but pressure independent for the lower densities and higher pressures. These results show that DFT methods may be capable of dealing with highly distended material with the proper modifications.

\textsuperscript{1}Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:30AM O2.00002 ABSTRACT WITHDRAWN

9:45AM O2.00003 International Shock-Wave Database: Current Status\textsuperscript{1}. PAVEL LEVASHOV, JIHT RAS — Shock-wave and related dynamic material response data serve for calibrating, validating, and improving material models over very broad regions of the pressure-temperature-density phase space. Since the middle of the 20th century vast amount of shock-wave experimental information has been obtained. To systemize it a number of compilations of shock-wave data has been issued by LLNL, LANL (USA), CEA (France), IPCP and VNIIEF (Russia). In mid-90th the drawbacks of the paper handbooks became obvious, so the first version of the online shock-wave database appeared in 1997 (http://www.fcp.ac.ru/rusbank). It includes approximately 20000 experimental points on shock compression, adiabatic expansion, measurements of sound velocity behind the shock front and free-surface-velocity for more than 650 substances. This is still a useful tool for the shock-wave community, but it has a number of serious disadvantages which can't be easily eliminated: (i) very simple data format for points and references; (ii) minimalist user interface for data addition; (iii) absence of history of changes; (iv) bad feedback from users. The new International Shock-Wave database (ISWdb) is intended to solve these and some other problems. The ISWdb project objectives are: (i) to develop a database on thermodynamic and mechanical properties of materials under conditions of shock-wave and other dynamic loadings, selected related quantities of interest, and the meta-data that describes the provenance of the measurements and material models; and (ii) to make this database available internationally through the Internet, in an interactive form. The development and operation of the ISWdb is guided by an advisory committee. The database will be installed on two mirrored web-servers, one in Russia and the other in USA (currently only one server is available). The database provides access to original experimental data on shock compression, non-shock dynamic loadings, isentropic expansion, measurements of sound speed in the Hugoniot state, and time-dependent free-surface or window-interface velocity profiles. Users are able to search the information in the database and obtain the experimental points in tabular or plain text formats directly via the Internet using common browsers. It is also possible to plot the experimental points for comparison with different approximations and results of equation-of-state calculations. The user can present the results of calculations in text or graphical forms and compare them with any experimental data available in the database. A short history of the shock-wave database will be presented and current possibilities of ISWdb will be demonstrated. Web-site of the project: http://iswdb.info.

\textsuperscript{1}This work is supported by SNL contracts # 1143875, 1196352.
10:15AM O2.00004 Physical State of Shocked Silica Aerogel. CARL GREEFF, JOHN BENAGE, KATERINA FALK, CHRISTOPHER FRYER, Los Alamos National Laboratory. THOMAS BOEHLY, CHAD MCCAUY, LLE, University of Rochester — We have performed laser driven shock experiments on silica aerogel of initial density 0.2 g/cc. These experiments employed streaked optical pyrometry as a temperature diagnostic. The Hugoniot states accessed have densities between the critical density and the crystal density, and temperatures of a few eV. These densities are high enough that bonding is non-negligible and the electronic spectrum is strongly modified from that of the constituent atoms. The temperature is high enough for electronic excitation to be important, but low compared to the full ionization limit. We examine the physical basis of Sesame equation of state models in this regime with special attention to uncertainty in the calculated temperature. We present new results from quantum molecular dynamics simulations for the structural and electronic properties in the shocked state, and use these results to improve the Sesame models.

10:30AM O2.00005 An Equation of State for Polyurea Aerogel Based on Multi-Shock Response

TARIQ ASLAM, Los Alamos National Laboratory, DIANA SCHROEN, Sandia National Laboratory, RICHARD GUSTAVSEN, BRIAN BARTRAM, Los Alamos National Laboratory — The methodology for making foamed Divinylbenzene (DVB) is described. For a variety of initial densities, foamed DVB is examined through multi-shock compression and release experiments. Results from multi-shock experiments on LANL’s 2-stage gas gun will be presented. A simple conservative Lagrangian numerical scheme, utilizing total-variation-diminishing interpolation and an approximate Riemann solver, will be presented as well as the methodology of calibration. It has been previously demonstrated that a single Mie-Gruneisen fitting form can replicate foam multi-shock compression response at a variety of initial densities; such a methodology will be presented for foamed DVB.

Wednesday, July 10, 2013 9:15AM - 10:45AM —
Session O3 NT.1 Novel Techniques: XRD
Fifth Avenue - Kyle Ramos, Los Alamos National Laboratory


JASON BAKER, HİPSEC, University of Nevada, Las Vegas and Los Alamos National Laboratory, RAVHI KUMAR, HİPSEC, University of Nevada, Las Vegas, NENAD VELISAVLJEVIC, Los Alamos National Laboratory, CHANGYONG PARK, CURTIS KENNEY-BENSON, YOSHIO KONO, HİPCAT, Geophysical Laboratory, Carnegie Institution of Washington, ANDREW CORNELIUS, HİPSEC, University of Nevada, Las Vegas, HİPSEC TEAM, LOS ALAMOS NATIONAL LABORATORY COLLABORATION, HİPCAT TEAM — We have designed a special sample cell assembly for simultaneous and in-situ x-ray diffraction, electrical resistance, and thermal conductivity measurements with Paris-Edinburgh type large volume press. Initial measurements have been performed on bismuth (Bi) to up to 7 GPa and 1000°C. Using Bi, which has a number of well-investigated solid-solid and solid-melt transitions, we have been able to demonstrate the feasibility of performing in-situ measurements and correlating the measured electrical-thermal-structural properties over a broad range of P-T conditions. The goal of developing this new multi-probe measurement capability is to further improve detection of the onset of solid-solid/melt transitions, relate structural and electrical properties of materials, determine changes in thermal conductivity at high P-T, and ultimately extend the technique for investigating other parameters, such as the Seebeck coefficient of thermolectric materials.


STEFAN TURNEAURE, Y.M. GUPTA, Wash. State. Univ. — X-ray diffraction (XRD) measurements at the impact surface, rather than the rear surface, of a shocked crystal have two important advantages: time-dependent material response can be directly monitored without the complications arising from wave reflections, and the shocked crystal may be examined in a constant state over a continuous range of peak stresses. Methods for obtaining XRD data at the impact surface of crystals impacting an X-ray window will be presented. An optical beam parallel to and passing in front of the impact surface is blocked by the projectile several hundred ns before impact providing a trigger (about 10 ns jitter) for the X-ray source and detector. The quantitative accuracy of the impact surface XRD method was established using Si(100) shocked elastically to 5.4 GPa. Impact surface XRD measurements are expected to play an important role at the Dynamic Compression Sector at the Advanced Photon Source. Work supported by DOE/NNSA.

9:45AM O3.00003 X-ray diffraction of shock driven phase transitions at the Linac Coherent Light Source

CYNTHIA BOLME, Los Alamos National Laboratory — The Linac Coherent Light Source provides a brilliant ultrafast pulse of hard x-rays that can be used to probe shocked compressible material dynamics. In recent experiments, we have employed a nanosecond laser to shock compress single crystal and polycrystalline silica and silicon, while examining the resulting material dynamics with x-ray diffraction using this x-ray free electron laser. Experimental results on phase transition dynamics will be presented.

10:15AM O3.00004 X-ray diffraction study of ramp-compressed Fe and MgO.

FEDERICA COPPARI, RAYMOND SMITH, JON EGGERT, RYAN RYGG, AM LYAZICKI, JAMES HAWRELIAK, DAMIEN HICKS, Lawrence Livermore National Laboratory, JIE WANG, THOMAS DUFFY, Princeton University, GILBERT COLLINS, Lawrence Livermore National Laboratory — The study of Fe and MgO under extreme conditions of pressure and temperature is of great relevance for a variety of fields ranging from basic science and high-pressure condensed matter to geophysics and planetary science. We used laser-driven ramp-compression to achieve 5 and 9 Mbar in Fe and MgO respectively and the structural evolution and transformations were documented by in-situ x-ray diffraction. Velocity interferometry was used to infer the pressure. We found that the hexagonal close-packed (hcp) structure of iron remains stable up to 5 Mbar with no significant change in the c/a ratio. A new phase of MgO was observed above 6 Mbar and it is consistent with the CsCl (B2) structure. The new polymorph remains stable up to 9 Mbar, the highest pressure reached in our experiments.

1 This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

10:30AM O3.00005 Femtosecond x-ray probes of shock-driven phase transitions in nanocrystals

AARON LINDENBERG, Stanford University / SLAC National Accelerator Laboratory, JOSH WITTENBERG, TIMOTHY MILLER, ELIZABETH SZAILGYI, Stanford University — We have utilized laser-generated shock waves to induce the wurtzite to rock salt structural phase transformation in cadmium sulfide nanorods, and have probed the resulting dynamics and transition state using femtosecond hard x-rays at the Linac Coherent Light Source (LCLS) in diffraction. Colloidal grown nanocrystals are an ideal model system with which to study phase transformations because they are defect-free single crystalline domains. Simulations of this transformation at the nanoscale have suggested a two-stage model consisting of a compression along the c-axis to form a 5 coordinate h-MgO intermediate followed by compressive shear along the a-axis, with the transformation rate limited by the shear step. We observe a stress-dependent transition path: At higher peak stresses, the majority of the sample is converted directly into the rock salt phase, with no evidence of an h-MgO intermediate prior to rock salt formation. At lower peak stresses, an h-MgO structure is observed. Additionally, the observed transformation stress is ~3GPa, significantly below the ~7GPa required under hydrostatic compression, confirming previous observations of shear catalyzed structural transformation under shock compression.

Wednesday, July 10, 2013 9:15AM - 10:45AM —
Session O4 TM Molecular Dynamics
Vashon - Ivan Oleynik, University of South Florida
9:15AM O4.00001 Atomic-Scale Theoretical Studies of Fundamental Properties and Processes in CHNO Plastic-Bonded Explosive Constituent Materials under Static and Dynamic Compression1. THOMAS D. SEWELL, Department of Chemistry, University of Missouri-Columbia — The results of recent theoretical atomic-scale studies of CHNO plastic-bonded explosive constituent materials will be presented, emphasizing the effects of static and dynamic compression on structure, vibrational spectroscopy, energy redistribution, and dynamic deformation processes. Among the chemical compounds to be discussed are pentaerythritol tetranitrate (PETN), hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX), nitromethane, and hydroxyl-terminated polybutadiene (HTPB). Specific topics to be discussed include pressure-dependent terahertz IR absorption spectra in crystalline PETN and RDX, microscopic material flow characteristics and energy localization during and after pore collapse in shocked (100)-oriented RDX, establishment of local thermodynamic temperature and the approach to thermal equilibrium in shocked (100)-oriented nitromethane, and structural changes and relaxation phenomena that occur in shocked amorphous cis-HTPB. In the case of shocked HTPB, comparisons will be made between results obtained using fully-atomic and coarse-grained (united atom) molecular dynamics force field models. Rather than attempting to discuss any given topic in extended detail, 3-4 vignettes will be presented that highlight outstanding scientific questions and the predictive methods and tools we are developing to answer them.

1The U. S. Defense Threat Reduction Agency and Office of Naval Research supported this research.

9:45AM O4.00002 Fast Quantum Molecular Dynamics Simulations of Simple Organic Liquids under Shock Compression, MARC CAWKWELL, ANDERS NIKLASSON, VIRGINIA MANNER, SHAWN MCGRANE, DANA DATTELBAUM, Los Alamos National Laboratory — The responses of liquid formic acid, acetonitrile, and nitromethane to shock compression have been studied using quantum-based molecular dynamics simulations with the self-consistent tight-binding code LATTE. Microcanonical Born-Oppenheimer trajectories with precise energy conservation were computed without relying on an iterative self-consistent field optimization of the electronic degrees of freedom at each time step via the Fast Quantum Mechanical Molecular Dynamics formalism [A. M. N. Niklasson and M. J. Cawkwell, Phys. Rev. B, 86, 174308 (2012)]. The input shock pressures required to initiate chemistry in our simulations agree very well with recent laser- and flyer-plate-driven shock compression experiments. On-the-fly analysis of the electronic structure of the liquids over hundreds of picoseconds after dynamic compression revealed that their reactivity is strongly correlated with the temperature and pressure dependence of their HOMO-LUMO gap.

10:00AM O4.00003 Quantum molecular dynamics simulations of the stability and reactivity of aluminum cyclopentadienyl clusters, SUFIAN ALNEMRAT, JOSEPH HOOPER, Naval Postgraduate School — We report ab initio quantum molecular dynamics simulations of the thermal stability and oxidation of aluminum-cyclopentadienyl clusters currently being considered as novel fuels or energetic materials. These clusters contain a small aluminum core surrounded by a single organic ligand layer. The aromatic cyclopentadienyl ligands form a very strong bond with surface Al atoms, giving rise to a stable organometallic cluster which crystallizes into a low-symmetry solid-state material. Our calculated heat of combustion per unit volume of this solid is quite high (60% that of pure aluminum) with reaction kinetics potentially much faster than nanoscale metals. Though this compound can be experimentally produced in small quantities, it is quite volatile. Here we report theoretical studies of the stability and decomposition of these passivated aluminum clusters in the presence of oxygen using Car-Parrinello molecular dynamics. We also consider alternate ligand forms which offer significantly increased steric protection or contain groups (such as fluorine) which may react with the metallic core.

10:15AM O4.00004 Reactive Molecular Dynamics Simulation of Hotspot Formation in Shock-Induced Void Collapse of Pentaerythritol Tetranitrate (PETN) , TZUYU SHAN, AIDAN THOMPSON, Sandia National Laboratories, New Mexico — We present results of molecular dynamics simulations of shocked hotspots formation in shock-induced void collapse of pentaerythritol tetranitrate (PETN) with the ReaxFF reactive force field. A supported shockwave is driven through a PETN crystal along the [110] orientation; void size and piston velocity are varied to investigate their effects on hotspot formation and detonation initiation. Formation of hotspots during void collapse is characterized by hotspot extent and maximum temperature. Results show hotspot extent is directly related to void size, but maximum temperature is only slightly affected. On the other hand, both hotspot extent and maximum temperature are strongly dependent upon piston velocity. Hotter and larger hotspots facilitate detonation and subsequent chemical reactions. During void collapse, NOX molecules are shown to be the dominant ejectile from the upstream void surface. Once the void is filled and the hotspot develops, formation of final products such as N2 and H2O become more dominant.

10:30AM O4.00005 Molecular dynamics simulation of the burning front propagation in PETN, ALEXEY YANILKIN, OLEG SERGEEV, All-Russia Research Institute of Automatics, COMPUTATIONAL MATERIALS SCIENCE TEAM — One of the models of detonation development in condensed explosives under shock loading is the concept of “hot spots.” According to this model, the reaction initially starts at various defects and inhomogeneities, where energy is localized during shock wave propagation. In such a region the exothermic reaction may start with heat yield sufficient for the ignition of the adjacent layers of matter. If the reaction propagates fast enough, the merging of the burning fronts from several hot spots may lead to detonation. So there is an interest in determining the burning propagation rate from the hot spot in various conditions. In this work we investigate the propagation of plane burning front from initially heated layer in PETN single crystal using molecular dynamics method with reaction force field (ReaxFF). It is shown that the burning rate depends on the direction in crystal. The kinetics of chemical transformations is considered, main reaction paths are determined. The dependence of the burning front propagation rate on the external pressure in the pressure range of normal to 30 GPa is calculated, it is shown that it grows linearly in the considered range from 50 m/s to 320 m/s. The results are compared with the data from experiments and quantum chemical calculations.

Wednesday, July 10, 2013 9:15AM - 10:45AM — Session O5 GP1: Geophysics IV Cascade I - Michael Brown, University of Washington

9:15AM O5.00001 EXAFS study of solid iron up to 560 GPa1. YUAN PING, F. COPPARI, D. HICKS, LLNL, B. YAAKOBI, LLE, D. FRATANDUONO, S. HAMEL, J. EGGERT, J. RYGG, R. SMITH, D. SWIFT, LLNL, T. BOEHLY, LLE, G. COLLINS, LLNL — Dynamic compression by multiple shocks is used to compress iron up to 560 GPa (5.6 Mbar), the highest solid-state pressure yet attained for iron in the laboratory. EXAFS (extended x-ray absorption fine structure) spectroscopy offers simultaneous density, temperature and local-structure measurements for compressed iron, providing highest-pressure data up to date for constraining solid state theory and evolution models for many newly discovered extra-solar terrestrial planets. The results show that the close-packed structure of iron is stable up to 560 GPa, the temperature at peak compression is significantly higher than expected from pure compressive work, and the strength of iron many times greater than expected from lower pressure data.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
9:30AM 05.00002 Single crystal crystallography of geomaterials at 100 GPa and above, LEONID DUBROVINSKY, BGI Bayeuth University, NATALIA DUBROVINSKAIA, ELENA BYKOVA, Bayeuth University, KONSTANTIN GLAZYRIN, TIZIANA BOFFA BALLARAN, CATHERINE MCCAMMON, ANASTASIA KANTOR, BGI Bayeuth University, MARCO MERLINI, MICHAEL HANFLAND, ALEXANDER CHUMAKOV, ESRF — Modern science and technology rely on the fundamental knowledge of matter that is provided by crystallographic studies. The most reliable information about crystal structures and their response to changes in pressure and temperature is obtained from single crystal diffraction experiments. Advances in diamond anvil cell techniques (DACs) and modern X-ray sources have increased the accessible pressure range for structural research up to several dozens of gigapascals. We have developed a methodology to perform single crystal X-ray diffraction experiments in double-side laser-heated DACs and demonstrated that the solution of crystal structures, their refinement, and accurate measurements of the thermal equation of state of metals, oxides, and silicates from single crystal diffraction data are possible in a megabar pressure range at temperatures of thousands degrees. Particular attention is paid to the in situ study of silicate perovskite (Pv) at extreme conditions. By tracking the changes of crystallographic parameters at pressures above 120 GPa and temperatures up to 2200 K, we found that (a) there is no a spin state crossover in ferric iron occupying the bicapped trigonal prism (“A”) crystallographic site, and (b) ferric iron does not enter the octahedral (“B”) site at any conditions of our experiments. We demonstrate that incorporation of ferric iron and aluminum significantly increases the compressibility of Pv and show that the oxidation state of iron is a critical parameter for interpretation of seismic tomography data.

9:45AM 05.00003 Evaluation of Elastic Properties of Iron in Diamond Anvil Cell by a Laser Ultrasonics Technique up to 52 GPa1, ALEXEY SEMENO, General Physics Institute, PAVEL ZININ, KATHERINE BURGESS, University of Hawaii, VITALI PRAKAPENKA, University of Chicago — In this report, we present results on measurements of shear and longitudinal wave velocities in iron under high pressure up to 52 GPa. The measurements were conducted using laser ultrasonics (LU) in diamond anvil cells (DAC), LU-DAC technique. The iron sample is attached to the lower diamond and separated from the upper diamond by NaCl. The way the sample is loaded in DAC allows measurements of acoustical wave velocities with two different configurations: acoustic waves propagated inside the specimen are excited and detected by a pump laser and a probe laser located (a) on the same side of the specimen or (b) on the opposite sides of the specimen. We found that the signals detected at the configuration (a) are similar to those measured without NaCl and show the arrival time of the longitudinal and shear waves. In addition to skimming and bulk acoustic modes observed and analyzed in a previous study, the detection of head waves is reported. In configuration (b), the signal shows arrival of the longitudinal wave and a set of the Lamb modes.

1) This work was supported by the NSF, Grant NO. EAR-1215796.

10:00AM 05.00004 In-situ XRD of iron at megabar pressures with short laser pulses, ZUZANA KONOPKOVA, DESY Photon Science, Notkestr. 85, 22607 Hamburg, Germany, ALEXANDER CONCHAROV, Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road NW Washington D.C., 20015, HANNS-PETER LIERMANN, DESY Photon Science, Notkestr. 85, 22607 Hamburg, Germany, WOLFGANG MORGENROTH, Inst. f. Geowissenschaften, Goethe Universität Frankfurt, D-60483 Frankfurt am Main, Germany, JAN TORSSEN DELITZ, DESY Photon Science, Notkestr. 85, 22607 Hamburg, Germany, VITALI PRAKAPENKA, Consortium for Advanced Radiation Sources, the University of Chicago, Chicago, Illinois, USA — Recent improvements and growing technical capabilities of synchrotron sources enable us to investigate matter on shorter time scales, partially bypassing problems with sample contaminations and reaching increasingly higher temperatures at higher pressures. High quality X-ray diffraction data are nowadays feasible to obtain in several tens of milliseconds thanks to the high photon flux and efficient large area detectors. In-situ XRD experiments were conducted at the Extreme Conditions Beamline, P02.2, PETRAIII, Hamburg. The short laser pulses keep the heating time at minimum, which proves to be less destructive to the diamonds and the sample. We have followed the above strategy to study iron at megabar pressures. Measuring diffraction of iron at Earth’s core conditions is technically difficult to achieve, which leads to contradictory results. We observe re-crystallization at highest temperatures and appearance of reflections with a large thermal shift. Further studies on melting and phase transitions will be conducted on iron and other metals in the near future.

10:15AM 05.00005 Melting and vibrational properties of planetary materials under deep Earth conditions, JENNIFER M. JACKSON, California Institute of Technology — The large chemical, density, and dynamical contrasts associated with the juxtaposition of a liquid iron-dominant alloy and silicates at Earth’s core–mantle boundary (CMB) are associated with a rich range of complex seismological features. For example, seismic heterogeneity at this boundary includes small patches of anomalously low sound velocities, called ultralow-velocity zones. Their small size (5 to 40 km thick) and depth (about 2800 km) present unique challenges for seismic characterization and geochemical interpretation. In this contribution, we will present recent nuclear resonant inelastic x-ray scattering measurements on iron-bearing silicates, oxides, and metals, and their application towards our understanding of Earth’s interior. Specifically, we will present measurements on silicates and oxide minerals that are important in Earth’s upper and lower mantles, as well as iron to over 1 megabar in pressure. The nuclear resonant inelastic x-ray scattering method provides specific vibrational information, e.g., the phonon density of states, and in combination with compression data permits the determination of sound velocities and other vibrational information under high pressure and high temperature. For example, accurate determination of the sound velocities and density of chemically complex Earth materials is essential for understanding the distribution and behavior of minerals and iron-alloys with depth. The high statistical quality of the data in combination with high energy resolution and a small x-ray focus size permit accurate evaluation of the vibrational-related quantities of iron-bearing Earth materials as a function of pressure, such as the Grünisen parameter, thermal pressure, sound velocities, and iron isotope fractionation quantities. Finally, we will present a novel method detecting the solid-liquid phase boundary of compressed iron at high temperatures using synchrotron Mössbauer spectroscopy. Our approach is unique because the dynamics of the iron atoms are monitored. This process is described by the Lamb-Mössbauer factor, which is related to the mean-square displacement of the iron atoms. We will discuss the implications of our results as they relate to Earth’s core and core-mantle boundary regions.

Wednesday, July 10, 2013 9:15AM - 10:45AM – Session O6 EM.1 Cook-off Cascade II - Marcia Cooper, Sandia National Laboratories

9:15AM O6.00001 Observations and Modeling of the Component Mechanisms in Deflagration, LAURA SMILOWITZ, BRYAN HENSON, DAVID OSCHWALD, ALAN NOVÁK, MATTHEW HOLMES, Los Alamos National Lab — We have used dynamic x-ray and proton radiography to observe the behavior of a series of HMX based energetic materials formulations undergoing thermal explosions. The result of these observations is a mechanism for deflagration based on both gas phase convective burning and solid phase conductive burning. The velocities for both the convective and conductive burns are tied together by the single combustion pressure driving both in a single experiment. The convective rate is directly measured as the burn front in the radiographs. The pressure associated with that rate is inferred from independently measured burn rate verses pressure data. This same pressure is then assumed to drive the conductive burning which begins as the convective burn front lights the material surface. Using a single, independently validated particle size distribution for damaged HMX, the combination of pressure driven convective lighting and conductive consumption is then calculated and compared to the measured transmission data sets. This same model with different initial pressurizations is used to successfully model deflagration in PBX9501, PBXN-9, and LX-07. In addition, a correlation between initial pressurization, convective/conductive velocity, and final “reaction violence” is observed. This leads us to the use of convective velocity as a metric for final energy release rate and therefore overall reaction violence.
9:30AM O6.00002 A thermodynamically based definition of fast verses slow heating in secondary explosives. BRYAN HENSON, LAURA SMILOWITZ, Los Alamos National Laboratory — The thermal response of energetic materials is often categorized according to the rate of heating as either fast or slow, e.g., slow cook-off. Such categorizations have most often followed some operational rationale, without a material based definition. We have spent several years demonstrating that for the energetic material octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) a single mechanism of thermal response reproduces times to ignition independent of rate or means of heating over the entire range of thermal response. HMX is unique in that bulk melting is rarely observed in either thermal ignition or combustion. We have recently discovered a means of expressing this mechanism for HMX in a reduced form applicable to many secondary explosives. We will show that with this mechanism a natural definition of fast versus slow rates of heating emerges, related to the rate of melting, and we use this to illustrate why HMX does not exhibit melting, and why a number of other secondary explosives do, and require the two separate categories.

9:45AM O6.00003 A Simple Model for the Pressure field from a Distribution of Hotspots. BRIAN LAMBOURN, HEATHER LACY, CAROLINE HANDLEY, AWE — At the APS SCCM in 2009, Hill, Zimmerman and Nichols showed how, assuming that burn fronts propagate at constant speed from individual point hotspots distributed randomly in a volume, the reaction rate history could then be determined. In this paper a simple analytic approximation is found for the time history of the pressure in the volume. Using acoustic theory, the time history of the pressure field for burning from a single spherical, isolated hotspot of finite radius is developed. Then at any point in the volume, the overall pressure history is determined from the sum of the pressure fields from all the individual hotspots. The results are shown to be in qualitative agreement with full mesoscale calculations of the reaction and burning from a finite size spherical hotspot.

10:00AM O6.00004 Microwave frequency material properties and ignition predictions of neat and plastic bound explosives. M. DAILY, S. SON, Purdue University, B. GLOVER, Los Alamos National Laboratory, L. GROVEN, Purdue University — Microwave energy has been considered for ignition, enhanced burning, and detection/defeat of energetic materials. However, the very limited data set of electromagnetic properties for both neat and plastic bound explosives has severely limited design and implementation of detection, defeat, and initiation devices. In this work, we report complex permittivity measurements for both neat and plastic bonded energetic materials such as HMX, RDX, PBX9501, etc. These measurements provide a new, more extensive set of self-consistent data that can be used to predict the response of such materials to electromagnetic energy. Using this data in conjunction with finite element software, a high localized field experimental microwave applicator was designed and microwave heating predictions were calculated. Predictions show the feasibility of heating low-loss energetic materials in such cavities with high local electric fields without the need for susceptor particles. For the plastic bound materials, the effect of the binder is presented, showing that electromagnetic energy is preferentially absorbed in the more absorptive binder, resulting in significant gradients within individual energetic crystals (e.g., HMX crystals in PBX 9501). These predictions are now being used to aid experimental work with the applicator cavity and have demonstrated the feasibility of volumetrically heating energetic materials in short time scales with low microwave power levels.

10:15AM O6.00005 Modeling the Effects of Confinement during Cookoff of Explosives. MICHAEL HOBBES, Engineering Sciences Center, Sandia National Laboratories, Albuquerque, NM 87111 — In practical scenarios, cookoff of explosives is a three-dimensional transient phenomenon where the rate limiting reactions may occur either in the condensed or gas phase. The effects of confinement are more dramatic when the rate-limiting reactions occur in the gas phase. Explosives can be self-confined, where the decomposing gases are contained within non-permeable regions of the explosive, or confined by a metal or composite container. Self-confinement is prevalent in plastic bonded explosives at full density. The time-to-ignition can be delayed by orders of magnitude if the reactive gases leave the confining apparatus. Delays in ignition can also occur when the confining apparatus has excess gas volume or ullage. Explosives with low melting points, such as trinitrotoluene (TNT) or cyclooctamethylene-trinitramine (RDX) are complex since melting and flow need to be considered when simulating cookoff. Cookoff of composite explosives such as Comp-B (mixture of TNT and RDX) are even more complex since dissolution of one component increases the reactivity of the other component. Understanding the effects of confinement is required to accurately model cookoff at various scales ranging from small laboratory experiments to large real systems that contain explosives.  

1Sandia National Laboratories is managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

Wednesday, July 10, 2013 9:15AM - 10:30AM — Session O7 EM.2 Nonconventional Energetics: Intermetallics

9:15AM O7.00001 Impact Ignition and Combustion Behavior of Amorphous Metal-Based Reactive Composites1, LORI GROVEN, BENJAMIN MASON, STEVEN SON, Purdue University — Recently published molecular dynamic simulations have shown that metal-based reactive powder composites consisting of at least one amorphous component could lead to improved reaction performance to amorphous materials having a zero heat of fusion, in addition to having high energy densities and potential uses such as structural energetic materials and enhanced blast materials. In order to investigate the feasibility of these systems, thermochemical equilibrium calculations were performed on various amorphous metal/metalloid based reactive systems with an emphasis on commercially available or easily manufactured amorphous metals, such as Zr and Ti based amorphous alloys in combination with carbon, boron, and aluminum. Based on the calculations and material availability material combinations were chosen. Initial materials were either mixed via a Resodyn mixer or mechanically activated using high energy ball milling where the microstructure of the milled material was characterized using x-ray diffraction, optical microscopy and scanning electron microscopy. The mechanical impact response and combustion behavior of select reactive systems was characterized using the Asay shear impact experiment where impact ignition thresholds, ignition delays, combustion velocities, and transient phenomenon where the rate limiting reactions may occur either in the condensed or gas phase. The effects of confinement are more dramatic when the rate-limiting reactions occur in the gas phase. Explosives can be self-confined, where the decomposing gases are contained within non-permeable regions of the explosive, or confined by a metal or composite container. Self-confinement is prevalent in plastic bonded explosives at full density. The time-to-ignition can be delayed by orders of magnitude if the reactive gases leave the confining apparatus. Delays in ignition can also occur when the confining apparatus has excess gas volume or ullage. Explosives with low melting points, such as trinitrotoluene (TNT) or cyclooctamethylene-trinitramine (RDX) are complex since melting and flow need to be considered when simulating cookoff. Cookoff of composite explosives such as Comp-B (mixture of TNT and RDX) are even more complex since dissolution of one component increases the reactivity of the other component. Understanding the effects of confinement is required to accurately model cookoff at various scales ranging from small laboratory experiments to large real systems that contain explosives.

1Funding from the Defense Threat Reduction Agency (DTRA), Grant Number HDTRA1-10-1-0119. Counter-WMD basic research program, Dr. Suhihiti M. Peiris, program director is gratefully acknowledged.

9:30AM O7.00002 Study of thermite mixtures consolidated by cold gas dynamic spray process. ANTOINE BACCIOCHINI, GEOFFREY MAINES, CHRISTIAN Poupard, MATEI RADULESCU, BERTRAND JODOIN, University of Ottawa, JULIAN LEE, DRDC — The present study focused on the cold gas dynamic spray process for manufacturing finely structured energetic materials with high reactivity, vanishing porosity, as well as structural integrity and arbitrary shape. The experiments have focused the reaction between the aluminum and metal oxides, such as Al-CuO and Al-MoO3 systems. To increase the reactivity, an initial mechanical activation was achieved through interrupted ball milling. The consolidation of the materials used the supersonic cold gas spray technique, where the particles are accelerated to high speeds and consolidated via plastic deformation upon impact, forming activated nano-composites in arbitrary shapes with close to zero porosity. This technique permits to retain the feedstock powder micro-structure and prevents any reactions during the consolidation phase. Reactivity of mixtures has been investigated through flame propagation analysis on cold sprayed samples and compacted powder mixture. Deglaffation tests showed the influence of porosity on the reactivity.

9:45AM O7.00003 ABSTRACT WITHDRAWN
10:00AM O7.00004 Shock compression response of Ti+B reactive powder mixtures\textsuperscript{1}, MANY GONZALES, ASHOK GURUMURTHY, GREGORY KEÑINDEY, ARUN GOKHALE, NAresh THADHANI, Georgia Institute of Technology — The shock compression response of Ti+B (1:2 Ti:B stoichiometric ratio) reactive powder mixtures at \( \sim 50\% \) theoretical material density (TMD) is investigated for shock pressures up to 5 GPa to investigate the possible shock-induced chemical reactivity of this highly exothermic mixture. The shock ablation is produced from instrumented parallel-plate gas-gun impact experiments on encapsulated powders using poly-vinylidene fluoride (PVDF) stress gauges to measure the input and propagated stress and wave speed in the powder. The shock compression regime is probed from crush-up to full density and onward to assess the potential onset of a shock-induced chemical reaction event in the powder mixture. A series of two-dimensional continuum meso-scale simulations on real and simulated microstructures are performed to predict the shock compression response and identify the meso-scale mechanisms that is essential for the so-called “ballotechnic” reaction. These meso-scale mechanisms are investigated through stereological evolution metrics that track particle interface evolution and their respective field variables. The suitability of the synthetic microstructural representations is evaluated by comparing the experimental and predicted pressure traces.

\textsuperscript{1}We gratefully acknowledge support and funding from DTRA through Grant No. HDTRA1-10-1-0038 and the National Defense Science and Engineering Graduate (NDSEG) Fellowship through the High Performance Computing and Modernization Office (HPCMO)

10:15AM O7.00005 Microstructural Effects on the Reactivity of Nano-Aluminum/Iodine (V) Oxide Films, B.K. LITTLE, E.J. WELLE, L.M. MARTINEZ, J.C. NITTINGER, M.B. BOGLE, S.B. EMERY, C.M. LINDSAY, A.M. SCHRAND, Air Force Research Laboratory, Munitions Directorate, Eglin AFB — Recent efforts investigating the self-ignition mechanism of nanoaluminum blended with iodine (V) oxide in the form of powders with and without additives suggests that ignition begins below the decomposition point of either reactant and takes place at the alumina shell surrounding the aluminum nanoparticles. As observed in previous studies of powder composites, microstructural features such as particle morphology are expected to strongly influence properties that govern the combustion behavior of this energetic material (EM). In this study, highly reactive composites containing amorphous and/or crystalline iodine oxide and micron/nano-sized Al was blended with an additive and deposited as films. Physiochemical techniques such as thermal gravimetric analysis, scanning calorimetry, X-ray diffraction, electron microscopy, high-speed imaging and planar doppler velocimetry were employed to characterize these EMs with emphasis on correlating the reaction rate (burn rate) with inherent microstructural features (porosity, thickness, TMD, etc.). This work was a continuation of efforts to probe the self-ignition mechanism of AI-iodine (V) oxide composites.

Wednesday, July 10, 2013 11:00AM - 12:15PM — Session P1 ME.3 Inelastic Deformation, Fracture, and Spall V Grand Ballroom I - Robert Rudd, Lawrence Livermore National Laboratory

11:00AM P1.00001 Gas Gun Driven Dynamic Fracture and Fragmentation of Ti-6Al-4V, DAVID JONES, DAVID CHAPMAN, DANIEL EAKINS, Institute of Shock Physics, Imperial College London — The dynamic fracture and fragmentation of a material is a complex late stage phenomenon occurring in many shock loading scenarios. Improving our predictive capability depends upon exercising our current failure models against new loading schemes and data. We present a series of experiments creating axially symmetric high strain rate (10\(^4\) s\(^{-1}\)) expansion of Ti-6Al-4V cylinders under controlled loading achieved using the ogive based gas gun technique. A steel ogive is located inside the cylinder, into which a polymer rod is launched. Deformation of the rod around the insert drives the cylinder into rapid expansion. This technique facilitates repeatable loading independent of the sample temperature and straightforward adjustment of radial strain rate. Expansion velocity was measured at multiple points along the cylinder outer wall using PDV. Two high speed imaging systems are used to track the overall expansion process to record strain at failure. Optical and SEM imaging is used to measure fragment size and mass distributions and examine the fracture surfaces to reveal the failure mechanism. For a peak radial strain rate of (1.1 \(\leq 0.1\) ) x 10\(^4\) s\(^{-1}\) strain localisation initiates on the outer surface at a radial strain of around 12\%, with cracks fully penetrating the cylinder wall at around 22\%. Hydrocode modelling has been carried out with very strong agreement in predicting the expansion velocity and profile but further work is needed to develop an accurate representation of the fracture and fragmentation.

11:15AM P1.00002 Understanding the micro-mechanics of spall initiation in titanium alloys, EUAN WIELEWSKI, Cornell University, GARETH APPLEBY-THOMAS, Cranfield University, PAUL HAZELL, The University of New South Wales — Significant progress has been made in understanding the effects of microstructural and micro-textural features on the mechanical behavior of titanium alloys at low strain rates. However, very little information is available in the literature on the effects of microstructure and micro-texture on the behavior of titanium alloys at high strain rates, particularly in terms of important failure mechanisms such as spall. In this study, the micro-mechanics of spall initiation in the titanium alloy, Ti-6Al-4V, was investigated via Backscatter Electron (BE) microscopy and Electron Back-Scatter Diffraction (EBSD) analysis of a recovered specimen from a typical plate-impact experiment. The analysis shows that spall initiates due to the nucleation of voids at the grain boundaries between plastically hard/soft grains and then propagates via the highly localized coalescence of the nucleated voids.

11:30AM P1.00003 The influence of the admixture of the fullerene C\(_{60}\) on strength properties of aluminum and copper under shock-wave loading, GALINA BEZRUCHKO, SERGEY RAZORENOV, Institute of Problems of Chemical Physics RAS, Chernogolovka, MIKHAIL POPOV, Technological Institute for Superhard and Novel Carbon Materials, Troitsk — Hugoniot elastic limit and dynamic (spall) strength measurements of pressed aluminum and copper samples with admixture of the fullerene C\(_{60}\) by 2-5 wt % under shock-wave loading were carried out. The peak pressure in shock-wave is equal to 6 GPa. The measurements of elastic-plastic and strength properties were based on the recording and the following analysis of the sample free surface velocity histories, recorded with VISAR laser-Doppler velocimeter. It was found, that the admixture of 5 wt % fullerene in aluminum samples lead to increasing of Hugoniot elastic limit for aluminum samples by a factor of ten. The copper samples with admixture of 2 wt % fullerene also demonstrated multiple increasing of the Hugoniot elastic limit in comparison with the commercial copper. The measured values of Hugoniot elastic limit were equal of 0.82-1.56 GPa for aluminum samples and 1.35-3.46 GPa for copper samples in dependence on their porosity. As it was expected, the spall strength of the samples with fullerene decreased about three times in comparison with the undoped samples as a result of influence of the solid fullerene particles which were concentrates of tension stresses in material in dynamic fracture process.

11:45AM P1.00004 Effect of severe plastic deformation on microstructure and mechanical properties of magnesium and aluminum alloys in wide range of strain rates, VLADIMIR SKRIPNYAK, EVGENIYA SKRIPNYAK, VLADIMIR VLADIMIROVICH SKRIPNYAK, IRINA VAGANOVA, NATALIYA SKRIPNYAK, National Research Tomsk State University — Results of researches testify that a grain size have a strong influence on the mechanical behavior of metals and alloys. Ultrafine grained HCP and FCC metals alloys present higher values of the strain strength than a corresponding coarse grained counterparts. In the present study we investigate the effect of grain size distribution on the flow stress and strength under dynamic compression and tension of aluminum and magnesium alloys. Microstructure and grain size distribution in alloys were varied by carrying out severe plastic deformation during the multiple-pass equal channel angular pressing, cyclic constrained groove pressing, and surface mechanical attrition treatment. Tests were performed using a VHS-Instron servo-hydraulic machine. Ultra high speed camera Phantom V710 was used for photo registration of deformation and fracture of specimens in range of strain rates from 0,01 to 1000 s\(^{-1}\). In dynamic regime UFG alloys exhibit a stronger decrease in ductility compared to the coarse grained material. The plastic flow of UFG alloys with a bimodal grain size distribution was highly localized. shear bands and shear crack nucleation and growth were recorded using high speed photography.
12:00PM P1.00005 Temperature effects on the low strain rate behaviour and piezoelectric charge production of PZT$^1$. AMNAH KHAN, JENS BALZER, WILLIAM PROUD, Institute of Shock Physics, Imperial College London — This presentation looks at the affect of varying strain rates and temperatures on the production of charge and fracture of the piezoceramic PZT. The samples are studied in the range of -80°C to +200°C whilst a range of strain rates ($10^{-4}$ s$^{-1}$ to $10^{-3}$ s$^{-1}$) is achieved using quasi-static Intron equipment, drop weight machines and compression Split Hopkinson Pressure Bars. Stress-strain data is obtained, and further analysis is made possible by the use of high-speed images.

$^1$Thanks to AWE for their funding and support

Wednesday, July 10, 2013 11:00AM - 12:30PM –
Session P2 CM Pressure Effects on Electronic Structure
Grand Ballroom II - Duck Young Kim, Carnegie Institute of Washington

11:00AM P2.00001 ABSTRACT WITHDRAWN –

11:15AM P2.00002 Pressure-Induced Valance change in Yterbium Organometallic Molecule Cp$^\ast_{x^2}$Yb(4,4′-Me$_2$-bipy) and Yterbium intermetallic YbCuGa, FARZANA NASREEN, DANIEL ANTONIO, ANDREW CORNELIUS, University of Nevada, Las Vegas, CORWIN H. BOOTH, Lawrence Berkeley National Laboratory, MILTON S. TORKIACHVILI, San Diego State University, San Diego, YU-MING XIAO, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois — We report on high pressure (0-15.3 GPa) x-ray absorption measurements in partial fluorescence yield mode (PFY-XAS) on two different kinds of Kondo systems: an organometallic molecular system Cp$^2$Yb(4,4′-Me$_2$-bipy) [Cp$^\ast$ = C$_2$Me$_5$, bipy = (NC$_2$H$_4$)$_2$ and Me = CH$_3$] and an intermetallic YbCuGa system. In the organometallic system, similar to the mixed valency in intermetallic Yb Kondo systems, the CASSCF calculations indicate that the intermediate valence in the ground state is due to a configuration interaction between the open-shell [4f$^{13/2}$] and the closed-shell [4f$^{11/2}$+$^{14}$m$^4$] spin-singlet states. Our analysis for Cp$^2$Yb(4,4′-Me$_2$-bipy) shows that with increase in pressure the overall valency increases from 2.77 at 2.7 GPa to 2.97 at 15.3 GPa. A considerable change in the slope of valency as function of pressure is observed at ~3.26 GPa suggesting a valence transition. The Kondo effect in such molecular compounds is intrinsic and provides a well defined nanoscale system to test the effect of size on the strongly correlated behavior. In the YbCuGa bulk system, the increase in pressure delocalizes the system and pushes it from valency of ~2.68 at ambient pressure to ~2.9 at 14.0 GPa.

11:30AM P2.00003 High-pressure Synchrotron Mössbauer Spectroscopy on Fe$_2$O$_3$, KARUNAKAR KOTHAPALLI, HIPSEC, Physics and Astronomy, University of Nevada, Las Vegas, NV, USA, TOMASZ KOLODZIEJ, AIGH University of Science & Technology, Krakow, Poland, EUNJA KIM, HIPSEC, Physics and Astronomy, University of Nevada, Las Vegas, NV, USA, ERCAN ALP, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA, BARBARA LAVINA, HIPSEC, Physics and Astronomy, University of Nevada, Las Vegas, NV, USA — Fe$_2$O$_3$ is a recently discovered compound belonging to the Fe-O binary system. We report the first insights on its properties as revealed by high pressure 57Fe Synchrotron Mössbauer Spectroscopy (SMS) performed at several different pressures in the range 0-48GPa. Fe$_2$O$_3$ first synthesized in the diamond anvil cell at a pressure of about 10 GPa and 1800 K, is a high pressure phase recoverable in ambient conditions. It crystallizes in the orthorhombic Cmmcm space group. The Fe atoms occupy three crystallographic positions – the 4a and 8f octahedral sites and 4c trigonal prism site. The SMS spectra could be fitted with just a single site and the Hyperfine Magnetic Field(HF) and Quadrupole Splittings(QS) were derived. The magnitudes of HF and QS indicate that the major contribution originates from high-spin Fe$^{3+}$ ions. The HF and QS parameters show a linear dependence in the region 10-48 GPa. A significant change in QS below 10 GPa suggests a valence transition. The Kondo effect in such molecular compounds is intrinsic and provides a well defined nanoscale system to test the effect of size on the strongly correlated behavior. In the YbCuGa bulk system, the increase in pressure delocalizes the system and pushes it from valency of ~2.68 at ambient pressure to ~2.9 at 14.0 GPa.

11:45AM P2.00004 Magneto-Structural coupling in compressed Manganese Oxide$^1$, ANTONIO M. DOS SANTOS, CHRIS A TULK, JAMIE J. MOLAISON, NEELAM PRADHAN, Neutron Sciences Directorate, ORNL Oak Ridge TN 37831-6475 — Transition metal oxides are relevant systems for the earth sciences as these are ideal model systems for Earth’s interior. In these systems, pressure increases the magnetic order 

$^1$This research at ORNL’s SNS was sponsored by the Scientific User Facilities Division, BES, from the U.S. Department of Energy.

12:00PM P2.00005 High Pressure Mössbauer Spectroscopic Studies on Narrow Band Co$_{1-x}$Fe$_x$S$_2$ Systems up to 9GPa, USHA CHANDRA, Department of Physics, University of Rajasthan, Jaipur 302004 India — Pyrite type 3d-transition metal disulfides exhibit a wide variety of interesting electrical and magnetic properties. Co$_2$S$_2$ is a ferromagnetic metal ordering ferromagnetically below ~120K while Fe$_2$S$_2$ is a narrow band gap magnetic semiconductor. Both Co and Fe are in low spin configuration. Formation of solid solutions between these two end members opens up the possibility of tuning the position of Fermi level in Co$_{1-x}$Fe$_x$S$_2$. Nano crystalline systems Co$_{1-x}$Fe$_x$S$_2$ ($x$=0.1 to 1.0) identically synthesized adopting solution technique were characterized by XRD, TEM. All the systems except $x$=0.8 showed nano sized particles. TEM micrographs taken for Co$_{0.2}$Fe$_{0.8}$S$_2$ system showed nano wires formation with SAED images indicating crystalline pattern. Electrical resistivity of bulk Ferromagnetic pyrite compounds Fe$_x$Co$_{1-x}$S$_2$ have shown an anomalous temperature dependence with increasing magnetic order below curie temperature due to the effect of a change in band width. Shift in the absorption edge with pressure in bulk pyrite Fe$_2$S$_2$ has been attributed to large compaction of S-S bonds in comparison to Fe-S bonds. $^{17}$Fe Mössbauer spectroscopic investigations on systems under high pressure are sensitive enough to probe variations in valence, spin configuration and site occupancy of Fe. The high pressure Mössbauer spectroscopic measurements using diamond anvil cell on nano crystalline Co$_{1-x}$Fe$_x$S$_2$ ($x$=0.2,0.5 and 0.8) would be reported to understand the pressure effect on band gap.
12:15PM P2.00006 Effect of Hydrostatic Pressure on Magnetic Caloric Effect of Charge- Orbital Order Perovskite manganite $Pr(Sr_{0.6}Ca_{0.4})_2Mn_2O_7$. ARUMUGAM S, THIYAGARAJAN R, MOHAN RADHEEP D, ESAKKI MUTHU S, Center for High Pressure Research, School of Physics, Bharathidasan University, Trichirappalli 620 024, India, GUOCHU DENG, EKATERINA POMJAKUSHINA, KAZIMIERZ CONDER, Laboratory for Developments and Methods, Paul Scherrer Institute, CH-5232 Villigen, Switzerland, CENTRE FOR HIGH PRESSURE RESEARCH TEAM, PAUL SCHERRER INSTITUTE COLLABORATION — The effect of hydrostatic pressure and magnetic field on magnetocaloric properties of half-doped bilayer manganite single crystal $Pr(Sr_{0.6}Ca_{0.4})_2Mn_2O_7$ has been investigated. The sample undergoes an antiferromagnetic (AF) transition at 103 K and a Charge-Orbital ordering (CO) at 179 K under ambient pressure with field of 0.5 T in c-axis. In CO ordered state, magnetization along c-axis shows the hysteresis which represents the first order phase transition and it is enhanced by both H and P. Simultaneously, magnetic caloric effect ($\Delta S_m$) and Relative Cooling Power (RCP) around $T_{CO}$ were increased by the application of the magnetic field and hydrostatic pressure. Although magnitude of $\Delta S_m$ is small compared to other conventional ferromagnetic manganites, this study may help to understand the effect of pressure on Magnetic Caloric Effect in antiferromagnetic manganites, especially, bilayer manganites. Further, RCP value gets increased in isothermal magnetization under P. Hence, $Pr(Sr_{0.6}Ca_{0.4})_2Mn_2O_7$ may be a potential candidate for magnetic refrigeration applications.

Wednesday, July 10, 2013 11:00AM - 12:15PM –
Session P3 NT.1 Novel Techniques: New Drives & Diagnostics
Fifth Avenue - Ray Smith, Lawrence Livermore National Laboratory

11:00AM P3.00001 Plane shock compression generators, utilizing convergence of conical shock waves, DMITRY NIKOLAEV, VLADIMIR TERNVOOI, ALEXANDER SHUTOV, VADIM KIM, Institute of problems of chemical physics RAS — The results of experimental testing of shock wave generators, based on Mach reflection of shock waves in a conical geometry, along with the results of numerical simulation will be presented. The hypervelocity shock in a layered cylindrical central body was produced by an impact of a converging conical flyer plate. Unlike in the designs proposed in the 80’s, a conical flyer plate was originating from initially cylindrical cavity liner in a cylindrical HE charge, was launched by a sliding detonation. This approach led to device simplification, since precision manufacturing of conical parts from metal and explosive is no longer required. The sequential HE charge detonation by a 234 points distributor was employed to vary the launch angle. Five various launch angles were tested; the dependence of parameters of shock wave in cylindrical PMMA core on launch angle was investigated; shock velocities of 14-19 km/s were obtained in a PMMA cylindrical core. This approach lead to device simplification, since precision manufacturing of conical parts from metal and explosive is no longer required. The sequential HE charge detonation by a 234 points distributor was employed to vary the launch angle. Five various launch angles were tested; the dependence of parameters of shock wave in cylindrical PMMA core on launch angle was investigated; shock velocities of 14-19 km/s were obtained in a PMMA cylindrical core. It was found that launch angles below 10° lead to the failure of the Mach reflection mode, while larger angles produced flat Mach disks with 16-17 mm diameter that could be utilized in various shock experiments.

11:15AM P3.00002 The ramp compression experiment with laser-driven reservoir target at Shenguang-III prototype facility, SHAN LIANQIANG, XIN JIANTING, SHUI MIN, GU YUQIU, Research Center of Laser Fusion, Chinese Academy of Engineering Physics — The quasi-isentropic compression of material can be obtained by the ramp wave loading of plasma jet produced by laser-driven reservoir target. The experiments were carried out on the high power laser facility of SG-III prototype using Al with direct-driven and indirect-driven method. The smooth and continuous speed history of free surface of specimen was recorded with a line-imaging velocity interferometer(VISAR). 16/26/36µm Al foil were compressed to more than 40 GPa with good planarity. The back-integrating method gave almost the same loading history for the three steps. 1µm Al backed by 500µm LiF were compressed to near 200GPa. The rise time of the load was about 10ns and the strain was about 10^5s^-1.

11:30AM P3.00003 Prospects for achieving high dynamic compression with low energy, MICHAEL ARMSMONG, JONATHAN CROWHURST, JOSEPH ZAUG, SORIN BASTEA, LLNL, ALEXANDER GONCHAROV, Carnegie Institution of Washington — Laser driven dynamic compression experiments may, in materials with picosecond equilibration times, be possible with orders of magnitude less drive energy than currently used. As we show, the compression energy for geometrical similar experiments varies as the third power of the time scale of compression. For materials which equilibrate and can be characterized on picosecond time scales, the compression energy can be orders of magnitude smaller than the 1–100 ns scale time scale of many current experiments. The use of substantially lower compression energy is a great practical advantage in such experiments, potentially enabling the observation of extreme states of matter with table top scale laser systems. We discuss prospects for realizing this scheme in practice. This work was performed in part under the auspices of the U.S. Department of Energy, National Laboratory and Laboratory directed Research and Development funding (11ERD039), as well as being based on work supported as part of the EFRel, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Grant No. DESC0001057.

11:45AM P3.00004 In-situ diffraction diagnostics in laser driven compression experiments, ANDREW HIGGINBOTHAM, University of Oxford — With the advent of increasingly powerful, and highly controllable laser systems, such as the National Ignition Facility (NIF) there is a peaked interest in the use of lasers to perform dynamic compression experiments relevant across a number of fields, from basic materials science to planetary physics. One key question in these experiments is how we gain information which takes us beyond a bulk understanding, to one which gives insight into the microstructure response during compression. In this talk we discuss recent developments in the field of in-situ x-ray diffraction. We will present the results of novel white light x-ray Laue experiments which demonstrate the measurement of both strain anisotropy and estimates of defect densities in-situ. In addition, a novel single photon energy dispersive diffraction geometry will be discussed which may prove to be ideally suited to the harsh environments characteristic of the NIF. We will also discuss the opportunities afforded by next generation light sources such as LCLS, and Europe’s XFEL project, which promise to provide techniques highly complimentary to those used at large scale laser facilities.

Wednesday, July 10, 2013 11:00AM - 12:30PM –
Session P4 TM Molecular Dynamics II
Vashon - Tommy Sewell, University of Missouri-Columbia

11:00AM P4.00001 PDPE Based Mesoscale Simulations of Shock Response of HE Composites, PARVEEN SOOD, SUNIL DWIVEDI, NARESH THADHANI, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, JOHN BRENNAN, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, YASUYUKI HORIE, (Retired) Air Force Research Laboratory, Eglin AF Base, FL 32555 — The dissipative and random force contributions of the PDPE method are used to account for the heat transport phenomena. The artificial viscosity terms are characteristic of the NIF. We will also discuss the opportunities afforded by next generation light sources such as LCLS, and Europe's XFEL project, which promise to provide techniques highly complimentary to those used at large scale laser facilities.

11:15AM P4.00002 Plane shock compression generators, utilizing convergence of conical shock waves, DMITRY NIKOLAEV, VLADIMIR TERNVOOI, ALEXANDER SHUTOV, VADIM KIM, Institute of problems of chemical physics RAS — The results of experimental testing of shock wave generators, based on Mach reflection of shock waves in a conical geometry, along with the results of numerical simulation will be presented. The hypervelocity shock in a layered cylindrical central body was produced by an impact of a converging conical flyer plate. Unlike in the designs proposed in the 80’s, a conical flyer plate was originating from initially cylindrical cavity liner in a cylindrical HE charge, was launched by a sliding detonation. This approach led to device simplification, since precision manufacturing of conical parts from metal and explosive is no longer required. The sequential HE charge detonation by a 234 points distributor was employed to vary the launch angle. Five various launch angles were tested; the dependence of parameters of shock wave in cylindrical PMMA core on launch angle was investigated; shock velocities of 14-19 km/s were obtained in a PMMA cylindrical core. It was found that launch angles below 10° lead to the failure of the Mach reflection mode, while larger angles produced flat Mach disks with 16-17 mm diameter that could be utilized in various shock experiments.

11:30AM P4.00003 Prospects for achieving high dynamic compression with low energy, MICHAEL ARMSMONG, JONATHAN CROWHURST, JOSEPH ZAUG, SORIN BASTEA, LLNL, ALEXANDER GONCHAROV, Carnegie Institution of Washington — Laser driven dynamic compression experiments may, in materials with picosecond equilibration times, be possible with orders of magnitude less drive energy than currently used. As we show, the compression energy for geometrical similar experiments varies as the third power of the time scale of compression. For materials which equilibrate and can be characterized on picosecond time scales, the compression energy can be orders of magnitude smaller than the 1–100 ns scale time scale of many current experiments. The use of substantially lower compression energy is a great practical advantage in such experiments, potentially enabling the observation of extreme states of matter with table top scale laser systems. We discuss prospects for realizing this scheme in practice. This work was performed in part under the auspices of the U.S. Department of Energy, National Laboratory and Laboratory directed Research and Development funding (11ERD039), as well as being based on work supported as part of the EFRel, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Grant No. DESC0001057.

11:45AM P4.00004 In-situ diffraction diagnostics in laser driven compression experiments, ANDREW HIGGINBOTHAM, University of Oxford — With the advent of increasingly powerful, and highly controllable laser systems, such as the National Ignition Facility (NIF) there is a peaked interest in the use of lasers to perform dynamic compression experiments relevant across a number of fields, from basic materials science to planetary physics. One key question in these experiments is how we gain information which takes us beyond a bulk understanding, to one which gives insight into the microstructure response during compression. In this talk we discuss recent developments in the field of in-situ x-ray diffraction. We will present the results of novel white light x-ray Laue experiments which demonstrate the measurement of both strain anisotropy and estimates of defect densities in-situ. In addition, a novel single photon energy dispersive diffraction geometry will be discussed which may prove to be ideally suited to the harsh environments characteristic of the NIF. We will also discuss the opportunities afforded by next generation light sources such as LCLS, and Europe’s XFEL project, which promise to provide techniques highly complimentary to those used at large scale laser facilities.

This work is supported in part by the DTRA Grant HDTRA1-12-1-0004 and ARL Grant W911NF-12-2-0053.
11:15AM P4.00002 Modeling the Shock Compression of Coarse-Grained RDX using Constant Energy Dissipative Particle Dynamics, JOSHUA D. MOORE, SERGEI IZVEKOV, JOHN K. BRENNAN, U.S. Army Research Laboratory, MARTIN LISAL, Institute of Chemical Process Fundamentals of the ASCR, v. v. i. — Mechanical simulation of energetic materials often incites responses over a wide range of spatial and temporal scales, with a strong dependence upon micron-scale defects. Modeling these materials atomistically remains a challenge due to the length and time scales required, as billions of molecules would be necessary to model micron-size defects. To overcome these challenges, we have implemented multiscale techniques to bridge the atomistic and mesoscale descriptions by coarse-graining RDX through a multiscale coarse-grain force-matching technique, resulting in a density-dependent potential. The resulting model reproduces several atomistic properties, but only those properties which depend on intermolecular interactions. Properties that depend on the coarse-grained intramolecular degrees-of-freedom (d.o.f.) are underestimated. Implementing traditional molecular dynamics to simulate the mechanical response of such models inevitably results in inaccurate energy and momentum exchange due to these unaccounted d.o.f. To correct this, we utilize the constant-energy Dissipative Particle Dynamics method (DPD-E), which provides a mechanism to account for all coarsened d.o.f. through the inclusion of a coarse-grain particle internal energy. This work presents results for shock simulations of RDX using DPD-E with results assessed by direct comparison to fully atomistic simulations.

11:30AM P4.00003 Laminar, cellular, transverse, and turbulent detonations in condensed phase energetic materials from molecular dynamics simulations, MIKLALI BUDZEVICH, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — The development of instabilities in condensed phase detonation is simulated using moving window molecular dynamics and a generic AB model of a high explosive. An initially planar detonation front with one-dimensional flow becomes unstable through the development of transverse perturbations. Highly inhomogeneous and complex two-dimensional cellular and transverse, and three-dimensional turbulent detonation structures were observed depending on the physico-chemical properties of the AB energetic material, sample geometry, and boundary conditions. The different regimes of condensed-phase detonation simulated by a moving window molecular dynamics technique exhibit structures, although at a much smaller scale, similar to those observed in gases and diluted liquids.

11:45AM P4.00004 Nano-scale spinning detonation in condensed phase energetic materials, VASILY ZHAKHOVSKY, MIKLALI BUDZEVICH, AARON LANDERVILLE, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Single- and multi-headed spinning detonation waves are observed in molecular dynamics simulations of a condensed phase detonation of an energetic material (EM) confined in round tubes of different radii. The EM is modeled using a modified AB Reactive Empirical Bond Order potential. The thermochemistry and reactive equation of state are varied by adjusting the barrier height for the exothermic reaction AB+B → A+BB. This allows us to study the evolution of the detonation-wave structure as a function of physico-chemical properties of the AB explosive. The detonation wave is found to exhibit a pulsating planar front in a tube of 8 nm radius, which later collapses due to the development of longitudinal perturbations. Upon increase of the tube’s radius to 16 nm, the detonation wave structure is stabilized through the development of a single-headed spinning detonation. The spinning detonation displays a four-wave configuration, including incident, oblique, transverse, and contact shock waves. The contact shock generated by a contact discontinuity is observed for the first time in our MD simulations. A multi-headed turbulent-like detonation structure develops within tubes of larger radii, and exhibit features similar to those observed in gases.

12:00PM P4.00005 Direct first-principles simulation of shock waves in silicon, OLIVER STRICKSON, University of Cambridge, EMILIO ARTACHO, University of Cambridge and CIC NanoGUNE — Density functional theory calculations of thousands of atoms are performed for the direct, non-equilibrium simulation of shock waves, using the SIESTA method and implementation of DFT. We perform a simulation of an elastic shock wave in silicon. We compare simulations using the direct method with equilibrium simulations of post-shock states found such that they lie on the Hugoniot locus, and simulations performed using existing empirical potentials for silicon. System size effects are addressed using conventional empirical interatomic potentials.

12:15PM P4.00006 The dissociation constant of water at extreme conditions, OTTO E. GONZALEZ-VAZQUEZ, International Center for Theoretical Physics “Abdus Salam” (ICTP), LUIGI GIACOMAZZI, International Center for Theoretical Physics “Abdus Salam” (ICTP), The International School for Advanced Studies (SISSA), C. PINILLA, SANDRO SCANDOLO, International Center for Theoretical Physics “Abdus Salam” (ICTP) — Only one out of 107 water molecules is dissociated in liquid water at ambient conditions, but the concentration of dissociated molecules increases with pressure ad temperature, and water eventually reaches a fully dissociated state when pressure exceeds 50-100 GPA and temperature reaches a few thousand Kelvin. The behavior of the dissociation constant of water (pKa) at conditions intermediate between ambient and the fully dissociated state is poorly known. Yet, the water pKa is a parameter of primary importance in the aqueous geochemistry as it controls the solubility of ions in geological fluids. We present results of molecular dynamics calculations of the pKa water at extreme conditions. Free-energy differences between the undissociated and the dissociated state are calculated by thermodynamic integration along the dissociation path. The calculations are based on a recently developed all-atom polarizable force-field for water, parametrized on density-functional theory calculations.

Wednesday, July 10, 2013 11:00AM - 12:30PM —
Session P6 EM.2 Shock Initiation Cascade II - Jared Gump, Naval Surface Warfare Center - Indian Head

11:00AM P6.00001 Experiment and Reactive-Burn Modeling in the RDX Based Explosive XTX 8004, CARL JOHNSON, MICHAEL MURPHY, RICHARD GUSTAVSEN, Los Alamos National Laboratory — XTX 8004 consists of 80 wt. % cyclotrimethylenetrinitramine (RDX), and 20 wt. % Sylgard 182, a silicone rubber used as a binder. Nominal density is 1.5 g/cm3. vs. 2-D experiments will be discussed. Calibration of Ignition & Growth to 1-D free surface velocity of the attenuator plate, and output of the acceptor charge was also measured using PDV. Parameterization of Ignition & Growth to 1-D order potential. The thermochemistry and reactive equation of state are varied by adjusting the barrier height for the exothermic reaction AB+B → A+BB. This allows us to study the evolution of the detonation-wave structure as a function of physico-chemical properties of the AB explosive. The detonation wave is found to exhibit a pulsating planar front in a tube of 8 nm radius, which later collapses due to the development of longitudinal perturbations. Upon increase of the tube’s radius to 16 nm, the detonation wave structure is stabilized through the development of a single-headed spinning detonation. The spinning detonation displays a four-wave configuration, including incident, oblique, transverse, and contact shock waves. The contact shock generated by a contact discontinuity is observed for the first time in our MD simulations. A multi-headed turbulent-like detonation structure develops within tubes of larger radii, and exhibit features similar to those observed in gases.
11:15 AM P6.00002 The increased shock sensitivity of PBX 9502 at high temperature. PHILIP RAE, EVA BACA, ANGELO CARTELLI, WX-6, LANL — It has been shown previously that the shock sensitivity of TATB based PBXs can be significantly increased at elevated temperature. In fact, some researchers have reported that at 250°C the Pop plot for LX-17 (a TATB based composition) overlays the Pop plot for room temperature PBX 9501 (an HMX based composition). The current study made use of the modified LANL small-scale gap test to investigate the shock sensitivity as a function of temperature. The modified gap test inputs an almost planar shock into the acceptor explosive rather than the more usual highly divergent one. This important change not only makes the geometry less sensitive to machining and assembly imperfections than a divergent version, but also allows accurate computer simulation using models calibrated to 1D Pop plot data. In these tests, samples of PBX 9502 were held at temperatures of 180, 200, 230 & 260°C for 30 minutes prior to firing the donor booster. As expected a significant increase in sensitivity was observed, but the material was not as sensitive as PBX 9501 even at 260°C. The method of performing these more complex high temperature gap tests and the accompanying computer modeling of the results will also be presented.

11:30 AM P6.00003 Experiments and numerical simulations of plate gap model for high energetic materials, SHIRO KUBOTA, TEI SABURI, YUJI OGATA, YUJI WADA, National Institute of Advanced Industrial Science and Technology, KUNITI TO NAGAYAMA, Kyushu University — The experimental system for this study consists of the pellet explosives and PMMA rings, PMMA pipe and booster explosive part. The pellets and the rings were alternately stacked in the PMMA pipe to make the system. The diameter of the pellet was 20 mm and the thicknesses were 10 or 5 mm. The thickness of the ring was varied to adjust the size of the air gaps between the pellets. The upper three pellet explosives were directly stacked without air gaps, and between the second and the third pellet, PVDF gauge was embedded to measure the arrival time of the detonation. The lower side pellet was put on the cylindrical stand made by PMMA, and the PVDF gauge was inserted between the pellet and PMMA to measure the arrival time of the detonation. Using the arrival times and a distance between two gauges, the average detonation velocity was estimated. The relationship between the size of the air gaps and detonation velocity was investigated. By changing both the gap size and the pellet, we consider that the system can roughly model the initial state of high energetic materials for qualitatively understanding of the initial state dependency. The detonation propagation processes in this system were simulated by our developed numerical code.

11:45 AM P6.00004 Effect of subcritical damage on sensitivity of a plastic bonded explosive, GEORGE SUNNY, CHAD RUMCHIK, JENNIFER JORDAN, THOMAS KRAWIETZ, Air Force Research Laboratory, Munitions Directorate — As energetic materials are subjected to increasingly more extreme environments, a more thorough understanding of the relationships between mechanical insult and changes in explosive sensitivity is desired. To that end, a Shock Wave Apparatus, originally developed at TDW (Schrobenhausen, Germany), has been employed to induce subcritical shocks of up to 0.7 GPa in a plastic bonded explosive sample while preserving the sample for further study. Changes in density due to the subcritical shocks are measured, and the sensitivity of the damaged explosive is determined through a TDW/AFRL Modified Gap Test configuration that allows the run-to-detonation (RTD) to be determined for a given shock loading. Changes in sensitivity are determined by comparing the RTD for each damaged sample with corresponding RTD for pristine (i.e. undamaged) samples. Confined Split-Hopkinson Pressure Bar experiments are also conducted in order to understand the effects of damage at lower strain-rates and pressures. Finally, the effects on sensitivity due to multiple shocks are also investigated in this study.

12:00 PM P6.00005 ABSTRACT WITHDRAWN —

12:15 PM P6.00006 Observation of sub-detonative responses in confined high density HMX-based PBXs, MALCOLM COOK, ANDREW WOOD, PHILIP OTTLEY, QinetiQ Ltd, PHIL CHEESE, MOD — This paper describes experiments and modelling aiming at understanding the behaviour of highly loaded (90%-95%) pressed HMX-based PBX compositions, when subjected to shock compression and ignition, by means of a propellant donor charge, under confinement. Such tests are routinely carried out in the UK on new formulations to determine their burn to violent reaction characteristics. The Bullseye propellant donor charge has been characterised in terms of pressure and temperature output. A range of tubes have been designed to examine the contribution of tube material properties (steel versus aluminium, 218.5MPa) and to examine the effect of reduced confinement (120MPa). For the reduced confinement scenario polycarbonate as well as steel and aluminium vessels have been designed which allow the reaction of the energetic material to be captured using high-speed video. In particular, tests carried out in the polycarbonate tubes have given a good insight of the processes occurring. Preliminary hydrocode modelling runs predicted an oscillating compressive wave in the explosive and considerable damage at either end of the explosive column. The latter leads to potential deconsolidation once the donor charge has burnt out allowing increased burning and violence.

1This work was undertaken as part of the MOD funded UK-Energetics research programme.

Wednesday, July 10, 2013 11:00 AM - 12:00 PM —

Session P7 Nonconventional Energetics: Shock Loading and Fragmentation Grand Crescent - Darla Thompson, Los Alamos National Laboratory

11:00 AM P7.00001 Shock Response and Explosive Launch of Compacted Reactive Material, JOHN D. MOLITORIS, ALEXANDER E. GASH, RAUL G. GARZA, FRANCO J. GAGLIARDI, JOSEPH W. TRINGE, JAN D. BATTEUX, P. CLARK SOUERS, Lawrence Livermore National Laboratory, HEAF TEAM — We have performed a series of experiments investigating the detailed dynamic response of compacted reactive material to shock and blast. Here a granular reactive formulation (Fe₃O₄/Al based thermite) was pressed into a solid cylinder of material and mated to a high-explosive charge of the same diameter. Detonation of the charge transmitted a shock wave to the thermite cylinder and imparted momentum launching it in the direction of the detonation. High-resolution time sequence radiography was used to image the dynamic response of the thermite. This technique allowed a detailed investigation of material deformation in addition to changes in the internal structure and indications of reactivity. The effect of variations in the initial density of the pressed thermite was also examined. We find that these pressed thermites behave much like solid metals during shock transit, then respond much differently.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
11:15AM P7.00002 Mechanisms of high strain, high strain rate plastic flow in the explosively driven collapse of Ni-Al laminate cylinders, KARL OLNEY, PO-HSUN CHIU, University of California, San Diego, ANDREW HIGGINS, MATTHEW SERGE, McGill University, GREGORY FRITZ, ADAM STOVER, Johns Hopkins University, DAVID BENSON, VITALI NESTERENKO, University of California, San Diego — Laminate materials composed of thin Ni and Al foils have shown promise as material systems used in reactive material applications due to the ability of the material to support a self-sustaining reaction between the Al and Ni layers. In addition to the traditional ignition methods, ignition may occur in the shear bands developed during mechanical loading. The thick-walled cylinder (TWC) technique was performed on samples of Ni-Al laminate materials with two different mesostructures; concentric and corrugated both constructed using alternating layers of Ni and Al thin foils on the order of 20-30 micron film thickness. These TWC experiments were performed to examine how these materials accommodated large plastic strain during the collapse which may be used to tailor reactivity in the material system. Large scale numerical simulations of these specimens with mesostructures digitized from the experimental samples were conducted to provide an insight into the mesoscale mechanisms of plastic flow during collapse of the thick walled laminate material during the explosive loading. Funding was provided by ONR MURI N00014-07-1-0740 (Program Officer Dr. Clifford Bedford)

11:30AM P7.00003 Fragmentation of Structural Energetic Materials: Implications for Performance1, BRADY AYDELOTTE, School of Materials Science and Engineering: Georgia Institute of Technology, CHRISTOPHER BRAITHWAITE, Fracture and Shock Physics Group: Cavendish Laboratory, NARESH THADHANI, School of Materials Science and Engineering: Georgia Institute of Technology — Fragmentation results for structural energetic materials based on intermetallic forming mixtures are reviewed and the implications of the fragment populations are discussed. Cold Sprayed Ni+Al and explosively compacted mixtures of Ni+Al+W and Ni+Al+W+Zr powders were fabricated into ring shaped samples and subjected to fragmentation tests. Ring velocity was monitored and fragments were soft captured in order to study the fragmentation process. It was determined that the fragments produced by these structural energetic materials are much smaller than those typically produced by ductile metals such as steel or aluminum. This has implications for combustion processes that may occur subsequent to the fragmentation process.

1 ONR/MURI grant No. N00014-07-1-0740. Dr. Cliff Bedford PM

11:45AM P7.00004 Fragmentation and Constitutive Response of Tailored Mesostructured Aluminum-Based Inert and Reactive Compacts2, ANDREW MARQUEZ, University of California San Diego, CHRIS BRAITHWAITE2, Cambridge University, TIMOTHY WEIHS, NICK KRYWOPUSK, DAVID GIBBINS, Johns Hopkins University, MARC MEYERS, University of California San Diego — The fragmentation and constitutive response of tailored aluminum-based compact is examined under dynamic conditions. Mesostructured compacts with tailored interfaces between the powders (with sizes of 40, 100, and 400 µm) were produced by swaging. In addition to these, reactive Ni-Al mixtures were prepared by the same technique; the Ni/Al layer thicknesses within the powders were varied to control the reaction rate between Ni and Al. The fragmentation produced in the explosively-driven rings expanded at a velocity of approximately 100 m/s was captured by high-speed photography. The fragment size distributions obtained varied widely and correlated with the interfacial strength of the compacts as well as with powder size. Experimental results are compared with fragmentation theories to characterize the behavior of reactive powders based on material mesostructure.

2 SMF Group, Cavendish Laboratory

Wednesday, July 10, 2013 1:45PM - 3:15PM  
Session Q1 ME.3 Inelastic Deformation, Fracture, and Spall VI  
Grande Ballroom I - Naresh Thadhani, Georgia Institute of Technology

1:45PM Q1.00001 Taylor Impact Tests on PBX Composites: Imaging and Analysis, DARLA GRAFF THOMPSON, RACCI DELUCA, Los Alamos National Laboratory — A series of Taylor impact tests were performed on three plastic bonded explosive (PBX) formulations: PBX 9501, PBXN-9 and HPP (propellant). The first two formulations are HMX-based, and all three have been characterized quasi-statically in tension and compression. The Taylor impact tests use a 500 psi gas gun to launch PBX projectiles (approximately 30 grams, 16 mm diameter, 76 mm long) at velocities as high as 215 m/s. Tests were performed remotely and no sign of ignition/reaction have been observed to date. High-speed imaging was used to capture the impact of the specimen onto the surface of a steel anvil. Side-view contour images have been analyzed using dynamic stress equations from the literature, and additionally, front-view images have been used to estimate a tensile strain failure criterion for initial specimen fracture. Post-test sieve analysis of specimen debris correlates fragmentation with projectile velocity, and these data show interesting differences between composites. Along with other quasi-static and dynamic measurements, these impact images and fragmentation data provide a useful metric for the calibration or evaluation of intermediate-rate model predictions of PBX constitutive response and failure/fragmentation. Intermediate-rate tests involving other impact configurations are being considered.

2:00PM Q1.00002 Shock and High Strain Rate Characterization of HTPB with Varying Plasticizer, DIDIER MONTAIGNE, CHRISTOPHER NEEL, Air Force Research Laboratory, Eglin AFB, FL 32542, PETER GOULD, QinetiQ, Bristol Business Park, Bristol BS16 1FJ, UK, CHRISTOPHER MOLEK, JENNIFER JORDAN, Air Force Research Laboratory, Eglin AFB, FL 32542 — Hydroxy-terminated polybutadiene (HTPB) has long been used as a binder in propellants and explosives. However, cured HTPB rubbery polyurethanes have not been characterized in a systematic fashion as function of plasticizer content. In this study, four isocyanate-cured HTPB variants with different amounts of plasticizer have been formulated. The materials were characterized using dynamic mechanical analysis and quasi-static and dynamic compression experiments. Additionally, the shock Hugoniots were measured on the two extremes of the material – no plasticizer and maximum plasticizer. The properties of the HTPB were predicted using the Porter-Gould model for polymers.

2:15PM Q1.00003 Polymorphism and Decomposition of HE Single Crystals: Insights from Static and Shock Compression Experiments, ZBIGNIEW DREGER, Washington State University — Understanding the reactive behavior of high explosive (HE) crystals at thermo-mechanical conditions generated by shock-waves is an important step toward understanding shock wave initiation of these crystals. Despite the significant differences in time scales and loading rates, static high pressure and high temperature (HP-HT) experiments can provide key results regarding structural and chemical processes in HE crystals at pressures and temperatures relevant to shock initiation. Here, we review recent progress in utilizing optical spectroscopy to understand molecular processes in HE crystals at static HP-HT conditions to gain insight into their shock initiation mechanisms. The relevant results obtained from static studies up to 20 GPa and 700 K on polymorphism, decomposition and phase diagrams will be presented for selected HE crystals: primarily for RDX and PETN, and initial results on DADNE. The significance of the stress state and the use of single crystals in these processes will be highlighted. Finally, we demonstrate that the static HP-HT results in conjunction with shock-wave experiments provide an important approach to elucidate processes related to the initiation of shocked HE crystals, including polymeric transitions, conformational changes, identification of crystal phases at decomposition, and mechanisms governing shock induced decomposition. Work was supported by DOE/NNSA and ONR/MURI, and carried out in collaboration with Y. M. Gupta.
2:45PM Q1.00004 Computational and Experimental Investigation of the Shock Compression Response of Cold-Rolled Ni/Al Multilayers, PAUL SPECHT, NARESH THADHANI, Georgia Institute of Technology, TIMOTHY WEIHS, The Johns Hopkins University — Heterogeneities at the meso-scale strongly influence the shock compression response of composite materials. In reactive material mixtures, such as Ni and Al, these heterogeneities greatly affect material mixing, heating, and activation, often initiating a reaction. Cold-rolled multilayered composites of Ni and Al provide a unique and potentially beneficial reactive material system, due to their full density, periodic layering, and intimate particle contacts. The shock-compression response of cold-rolled Ni/Al multilayers was investigated under uniaxial strain loading conditions using plate-impact experiments. Time-resolved diagnostics, including VISAR, PDV, and PVDF stress gauges, were used to obtain the equilibrium Hugoniot response of the multilayers. The experimental results were coupled with a computational investigation using the multi-material, finite-volume, Eulerian hydrocode CTH, developed by Sandia National Laboratories. The computations employed real, heterogeneous microstructures, obtained from optical microscopy, enabling their correlation with the experimental results to provide validation of the models and computational method used for describing the response of the cold-rolled Ni/Al multilayers. Research funded by ONR/MURI grant No. N00014-07-1-0740.

3:00PM Q1.00005 Prediction of Probabilistic Ignition Behavior of PBXs from Microstructural Stochasticity, SEOKPUM KIM, ANANDA BARUA, Georgia Institute of Technology, YASUYUKI HORIE, Air Force Research Lab, Eglin AFB, FL, MIN ZHOU, Georgia Institute of Technology — A novel approach is developed to computationally predict and quantify the stochasticity of the ignition process in polymer-bonded explosives (PBXs) under impact loading. The method involves subjecting sets of statistically similar microstructure samples to identical overall loading and characterizing the statistical distribution of the ignition response of the samples. The focus of the analyses is exclusively on the influence of microstructure geometry variations on the critical time to ignition at given load intensity and the critical impact velocity below which no ignition occurs. Results show that the probability distribution of the time to criticality follows the Weibull distribution. The quantification of this probability distribution as a function of microstructural attributes including grain volume fraction, grain size and specific binder-grain interface area along with the stochastic variations of these attributes within each set of samples yields relations that reveal microstructural parameters that play dominant roles in determining the ignition behavior of the materials. In particular, it is found that the specific interfacial area directly influences the critical time to ignition and the critical impact velocity below which no ignition is observed.

Wednesday, July 10, 2013 1:45PM - 3:15PM – Session Q2 CM.2 Phase Transitions: Superconductivity

1:45PM Q2.00001 Fe moments in the pressure-induced collapsed tetragonal phase of (Ca_{0.67}Sr_{0.33})Fe_2As_2, JASON JEFFRIES, NICH A BUTCH, JOSEPH BRADLEY, Lawrence Livermore National Laboratory, YUMING XIAO, PAUL CHOW, Carnegie Institute of Washington, SHANTA SAHA, KEVIN KIRSHENBAUM, JOHNPIERRE PAGLIONE, University of Maryland — The tetragonal AFe_2As_2 (A=alkaline earth element) family of iron-based superconductors exhibits magnetic order at ambient pressure and low temperature. Under pressure, the magnetic order is suppressed, and an isostructural volume collapse is induced due to increased As-As bonding across the mirror plane of the structure. This collapsed tetragonal phase has been shown to support superconductivity under some conditions, and theoretical calculations suggest an unconventional origin. Theoretical calculations also reveal that enhanced As-As bonding and the magnitude of the Fe moments are correlated, suggesting that the Fe moments can be quenched in the collapsed tetragonal phase. Whether the Fe moments persist in the collapsed tetragonal phase has implications for the pairing mechanism of the observed pressure-induced superconductivity in these compounds. We will present pressure-dependent x-ray emission spectroscopy (XES) measurements that probe the Fe moments through the volume collapse transition of (Ca_{0.67}Sr_{0.33})Fe_2As_2. These measurements will be compared with previously reported phase diagrams that include superconductivity. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the US Department of Energy (DOE), National Nuclear Security Administration under Contract No. DE-AC52-07NA27344.

2:00PM Q2.00002 Enhancement of Superconductivity of Beryllium at High Pressure, KATSUYA SHIMIZU, KAZUHISA KUBOTA, TAKAKIHO KATSOUKA, ATSUSHI MIYAKE, MASAFUMI SAKATA, YUKI NAKAMOTO, Osaka University, YASUO OHISHI, JASRI/SPring-8 — Among elements shows superconductivity at high pressure, some elements show the large enhancement of the transition temperature (Tc) at higher pressures. In the case of lithium, the Tc at ambient pressure is 0.4 mK which is the lowest observed value in whole elements, however, is enhanced by pressure up to near 20 K [1]. And calcium, which is on the same group II and not superconductive at ambient pressure, shows the highest Tc of elements at 29 K under pressure [2]. Then we focused on high pressure behavior at high pressure (P<50 GPa) and low temperature (T<100 mK) and found that the Tc rose up to few Kelvin at pressure above 20 GPa and reached up to 3.7 K at 30 GPa. In this pressure range the hcp crystal structure is stable at room temperature. We performed a powder X-ray diffraction measurement at room temperature and low temperature in BL10XU at SPring-8 and found a discontinuous change in c/a ratio at around 25 GPa.[1] K. Shimizu, H. Ishikawa, D. Takao, T. Yagi and K. Amaya, Nature 419, 597-599 (2002).[2] M. Sakata, Y. Nakamoto, and K. Shimizu, Phys. Rev. B 83, 220512 (2011).[3] K. Nakano, Y. Akahama and H. Kawamura, J. Phys.: Condens. Matter 14, 10569–10573 (2002).

2:15PM Q2.00003 Insulator-metal transitions and superconductivity in solids at high pressures, RANGA DIAS, Institute for Shock Physics and Department of Physics, Washington State University, Pullman, Washington 99164 — Under high pressure, simple molecular solids transform into non-molecular (extended) solids as compression energies approach the energies of strong covalent bonds in constituent chemical species. As a result, it is common to observe the transformation of molecular solids into more compact extended structures with strong non-linear second harmonic optical properties, electric and optical conductivities, and magnetic properties of condensed-matter systems. Carbon dioxide, for example, exhibits a richness of high-pressure polymorphs with a great variety in intermolecular interactions, chemical bonding, and crystal structures. Thus, group IV sulfides, in comparison with their chemical analog CO_2, provide opportunities to exploit the relationship between the structural phase transition, electronic metalization, and superconductivity. We present integrated spectral, structural, resistance, and theoretical evidence for several systems of simple molecular group IV sulfides that undergo pressure-induced electronic phase transitions to novel metallic, magnetically ordered, and/or superconducting states.

1The work has been performed in support of NSF-DMR (Grant No. 0854618 and 1203834)
2:45PM Q2.00004 High-pressure studies for hydrogen-doped LaFeAsO$_{1-x}$H$_x$ and SmFeAsO$_{1-x}$H$_x$. HIROKI TAKAHASHI, TAKAHIRO TOMITA, HIDETO SOEDA, Nihon University, SISI IIMUMA, TAKU HANNA, YOSHINORI MURABA, SATORU MATSUSHI, HIDEO HOSONO, Tokyo Institute of Technology — Iron-based superconductor LaFeAsO$_{1-x}$F$_x$ shows the conventional superconducting dome in an $x$-$T$ phase diagram with a maximum $T_c$ of 26 K at $x=0.1$. However, the over-doped region has not been investigated, because of the poor solubility of fluorine above $x=0.2$. Recently, hydrogen was doped for LaFeAsO$_{1-x}$H$_x$ above $x=0.5$. It is interesting that LaFeAsO$_{1-x}$H$_x$ exhibits the second superconducting dome in the over-doped region ($0.2 < x < 0.5$) with a maximum $T_c$ of 36 K, in addition to the conventional dome. Since large enhancement of $T_c$ under high pressure was reported for LaFeAsO$_{1-x}$F$_x$, it is intriguing to study the superconducting properties in LaFeAsO$_{1-x}$H$_x$ ($x>0.2$) under high pressure. Marvelous results that $T_c$ of $x=0.2$, which corresponds to the ravine between two domes, is enhanced largely from 18 K to 52 K with pressure of 6 GPa are obtained from resistivity measurements. These results are compared with the superconducting properties under high pressure of SmFeAsO$_{1-x}$H$_x$.

3:00PM Q2.00005 Uniaxial pressure effect of Metal-Insulator Transition ($T_{MI}$) in oriented Sm$_{0.55}$(Sr$_{0.5}$Ca$_{0.5}$)$_{0.45}$MnO$_3$. SONACHALAM ARUMUGAM, D. MOHAN RADHEEP, Centre for High Pressure Research, Bharathidasan University, P. SARKAR, P. MANDAL, Saha Institute of Nuclear Physics, Kolkata, ARUMUGAM TEAM, PRABHAT MANDAL COLLABORATION — Perovskite type manganites $R_{1-x}A_x$MnO$_3$ ($R$: rare earth ions, $A$: alkaline earth ions) exhibit various fundamental phenomena like colossal magnetoresistance (CMR), phase separation, and first-order ferromagnetic (FM) to paramagnetic (PM) phase transition etc. Similar to CMR, piezoresistance (PR), the change in electrical resistance in response to external pressure, can also be important parameter for various technological applications. Several studies shows that the order of phase transition can be changed either by applying external perturbations like magnetic field, pressure ($P$), etc. or internally like doping etc. SSMCO single crystal was grown using floating zone technique and the quality was carefully checked and aligned along the $c$-axis as well as $ab$-plane. We have investigated the effect of uniaxial pressure ($P$) on electrical resistivity along the $ab$-plane and $c$-axis in a single crystal of SSMCO. A huge $P_{MI}$ of $10^7$% at $P=90$ MPa and a remarkable increase ($\sim 79$ K/GPa) of $T_{MI}$ have been observed with the application of $P$ (c-axis), while $T_{MI}$ decreases at the rate of $\sim 77$ K/GPa for $P \perp c$ axis. These values of $PR$ and $dT_{MI}/dP$ are much larger than those observed in other perovskite and bilayer manganites. Hence, these materials may be used for various technological applications.

Wednesday, July 10, 2013 1:45PM - 2:45PM — Session Q4 NT.1 Superhard Materials II Vashon - Peter Pauzauskie, University of Washington

1:45PM Q4.00001 Synthesis and Characterization of Low-Cost Superhard Transition-Metal Borides, RICHARD KANER, Department of Chemistry and Biochemistry, Department of Materials Science and Engineering, and California NanoSystems Institute, UCLA — The increasing demand for high-performance cutting and forming tools, along with the shortcomings of traditional tools materials such as diamond (unable to cut ferrous materials), cubic boron nitride (expensive) and tungsten carbide (relatively low hardness), has motivated the search for new superhard materials for these applications. This has led us to a new class of superhard materials, dense refractory transition-metal borides, which promise to address some of the problems of conventional superhard materials. For example, we have synthesized rhenum diboride (ReB$_2$) using arc melting at ambient pressure. This superhard material shows an excellent electrical conductivity and superior mechanical properties, including a Vickers hardness of 48.0 GPa (under an applied load of 0.49 N). To further increase the hardness and lower the materials costs, we have begun exploring high boron content superhard borides including tungsten tetaboride (WB$_4$). We have synthesized WB$_4$ by arc melting and studied its hardness and high-pressure behavior. With a similar Vickers hardness (43.3 GPa under a load of 0.49 N) and bulk modulus (326-339 GPa) to ReB$_2$, WB$_4$ offers a lower cost alternative and has the potential to be used in cutting tools. To further enhance the hardness of this superhard metal, we have created the binary and ternary solid solutions of WB$_4$ with Cr, Mn and Ta, the results of which show a hardness increase of up to 20 percent. As with other metals, these metallic borides can be readily cut and shaped using electric discharge machining (EDM).

2:15PM Q4.00002 Novel metal borides: structure, high-pressure behavior and properties. ELENA BYKOOVA, Bayerian Research Institute of Experimental Geochemistry and Geophysics, University of Bayreuth, HUIYANG GOU, Material Physics and Technology at Extreme Conditions, University of Bayreuth — Iron-based superconductors show a second superconducting dome in the over-doped region ($0.2 < x < 0.5$) with a maximum $T_c$ of 36 K, in addition to the conventional dome. Since large enhancement of $T_c$ under high pressure was reported for LaFeAsO$_{1-x}$F$_x$, it is intriguing to study the superconducting properties in LaFeAsO$_{1-x}$H$_x$ ($x>0.2$) under high pressure. Marvelous results that $T_c$ of $x=0.2$, which corresponds to the ravine between two domes, is enhanced largely from 18 K to 52 K with pressure of 6 GPa are obtained from resistivity measurements. These results are compared with the superconducting properties under high pressure of SmFeAsO$_{1-x}$H$_x$.

2:30PM Q4.00003 New hybrid materials from compressing intercalated fullerides, MINGGUANG YAO, BINGBING LIU, WEN CUI, JUNPING XIAO, State Key Laboratory of Superhard Materials, Jilin University — Upon compression, molecular crystal undergoes complicated transformations, including the crystal structure, molecular morphology, and inter- and intra-molecular bonding. Here, we studied a series of two-component fullerides composed of C60 molecules and various dopants under pressure and demonstrate the effect of the dopants on the structural evolution of C60s upon compression. C60 molecules are found to behave similarly, deformed and even collapsed at high pressures, while the different interactions between the intercalated dopants and C60s result in different properties of the phases formed at high pressure. A class of new hybrid structures has been fabricated, in which several superhard phases have been discovered. The underlying mechanism for the superhard phase formation has been further uncovered.

Wednesday, July 10, 2013 1:45PM - 3:15PM — Session Q5 EM.1 Detonation I Cascade I - Tariq Aslam, Los Alamos National Laboratory

1This work was supported by the National Basic Research Program of China (2011CB808200), the NSFC (10979001, 11001405, 51025206, 51032001, 21073071), and the Cheung Kong Scholars Programme of China.
1:45PM Q5.00001 The influence of small additions of diethylenetriamine on the detonation waves stability for nitromethane/acetone solution. VALENTINA MOCHALOVA, ALEXANDER UTKIN, IPCP RAS — Instability of detonation front in nitromethane/acetone (NM/A) solution was observed in our previous work: at 10% of acetone the amplitude of heterogeneities was about 20 µm and at 20% of acetone this size was 50 µm. It is known that small additions of diethylenetriamine (DETA) considerably increase the initial rate of chemical reaction in detonation wave for NM. It was expected that DETA influences on the stability of detonation waves in NM/A solution too. To investigate this phenomenon laser interferometer VISAR was used for recording of particle velocity profiles in detonation waves for NM/A. It was found that at addition of 0.5% DETA to NM/A 90/10 the oscillations in velocity profile decrease in several times. And at 1% DETA the profile is smooth, i.e. the heterogeneities disappear and detonation wave becomes steady-state. In NM/A 80/20 at addition of 5% DETA the heterogeneities size is reduced by the order. The increase of detonation wave velocity of NM/A more than 1% was observed at small concentrations of DETA. Thus it was found that small additions of DETA to NM/A solution with unstable detonation front result not only in decrease heterogeneities size but in their disappearance and stabilization of detonation waves.

2:00PM Q5.00002 Detonation Reaction Zone Measurements of PBX 9501 and PBX 9502. SAMUEL VINCENT, MARK SHORT, SCOTT JACKSON, Los Alamos National Laboratory — Explosives are often confined by inert materials. During detonation, the high pressures associated with the detonation reaction zone and expansion of products induce motion in the confiner. Classical programmed burn models for conventional high explosives (CHEs) performance do not aim to accurately capture the contribution to CHE drive from the short (100-200 micron) detonation reaction zone, as the drive is dominated by expansion of detonation products. However, the reaction zone lengths of insensitive (millimeter-scale) and non-ideal explosives (millimeter-to-centimeter-scale) are long enough that a significant contribution to the HE work on the confiner occurs within the reaction zone. Thus accurate prediction of the reaction zone flow structure and mechanical state is crucial to accurately model the motion of confiners driven by insensitive and non-ideal explosives. In this work, we have measured particle velocity profiles of detonation reaction zones in PBX 9501 and PBX 9502 slab geometries at the breakout surface using PDV imaging through LiF windows. We compare this data to predictions in the slab geometry using the Wescott-Stewart-Davis reactive burn model and comment on the model performance.

2:15PM Q5.00003 CREST Modelling of PBX 9502 Corner Turning Experiments at Different Initial Temperatures. NICHOLAS WHITWORTH, AVE — Corner turning is an important problem in regard to detonation wave propagation in TATB-based explosives. Experimentally, a sudden change in direction of the propagating wave, such as turning a sharp corner, can result in dead-zones being left behind in the corner turn region, with the observed behaviour being particularly sensitive to the initial temperature of the explosive. In this paper, the entropy-dependent CREST reactive burn model is used to simulate corner turning experiments on the TATB-based explosive PBX 9502. Calculated results of double cylinder tests at three different initial temperatures (-54°C, 25°C, and 75°C), and a “hockey puck” experiment at ambient temperature, are compared to the corresponding test measurements. The results show that the model is able to: (i) calculate persistent dead-zones in PBX 9502 without recourse to any shock desensitisation treatment, and (ii) predict changes in corner turning behaviour with initial temperature using one set of coefficients.

2:30PM Q5.00004 Understanding Detonation Corner Turning within Ultra-Fine TATB: Measurements and Modeling. JOSE SINIBALDI, PETER VITELLO, CHADD MAY, Lawrence Livermore National Laboratory — Detonation corner turning within insensitive high explosives has demonstrated difficulties as the insensitivity of the high explosive increases. Experiments tend to report breakout profiles, which show times of arrival of the detonation wave at the surface of the IHE charge. Although, various reactive flow models are able to predict these breakout profiles, none of these models agree perfectly with each other. Models predict major differences in pressure profiles and in the internal detonation wave propagation characteristics. Thus, the objective of this study was to provide detailed accounts of the wave propagation within an ultra-fine TATB charge, through the use embedded fiber-optic diagnostics that allowed measuring the detonation wave propagation within the ultra-fine TATB charges. In addition, these experiments were also instrumented at multiple points with Photonic Doppler Velocimetry to provide dynamic pressure profiles at the hemispherical surface; and orthogonal streak cameras to provide the conventional breakout profiles. Comparisons between experimental data and simulation results using a high resolution reactive flow model for ultra-fine TATB will be presented.

1:45PM Q5.00005 On the verification and validation of detonation models. JAMES QUIRK, Los Alamos National Laboratory — This talk will consider the verification and validation of detonation models, such as Wescott-Stewart-Davis (Journal of Applied Physics, 2005), from the perspective of the American Institute of Aeronautics and Astronautics policy on numerical accuracy (AIAA J. Vol. 36. No. 1, 1998). A key aspect of the policy is that accepted documentation procedures must be used for journal articles with the aim of allowing the reported work to be reproduced by the interested reader. With the rise of electronic documents, since the policy was formulated, it is now possible to satisfy this mandate in its strictest sense: that is, it is now possible to run a computational verification study directly in a PDF, thereby allowing a technical author to report numerical subtleties that traditionally have been ignored. The motivation for this document-centric approach is discussed elsewhere (Quirk2003, Adaptive Mesh Refinement Theory and Practice, Springer), leaving the talk to concentrate on specific detonation examples that should be of broad interest to the shock-compression community.

Wednesday, July 10, 2013 1:45PM - 3:15PM — Session Q6 TM Molecular Dynamics III — Cascade II - Roman Martyonak, Comenius University

1:45PM Q6.00001 Evaluation of metastable region boundaries for liquid and solid states in MD simulations. GENNADY IONOV, VLADIMIR DREMOV, ALEKSEY KARAVAIEV. Zababakhin All-Russia Research Institute of Technical Physics, Russian Federal Nuclear Center, SERGEY PROTSENKO, VLADIMIR BAIDAKOV, AZAT TIPEEV, of Thermal Physics, Russian Academy of Sciences, Ural Branch, 106, Amundsen Street — An automatic method based on MD calculations was developed for detecting and tracing the boundaries of metastable states of superheated crystal and supercooled liquid. The main criterion of the detection of early nucleation of new phase is the self-diffusion coefficient temperature dependence. The scanning for nucleation events is performed at continuous temperature change. The set of independent nucleation events at a given pressure allows evaluation of temperature dependence of specific nucleation frequency. The collection of a large number of these calculations allows accurate approximation of the specific nucleation frequency surfaces in both directions of phase transition. These surfaces provide an opportunity to estimate the behavior of the free energy in the region between overheating and overcooling surfaces. In addition, dependence of nucleation frequency on pressure and temperature provides an opportunity to integrate the probability of nucleation under dynamic loading and subsequent release and thus to determine the likelihood of the crystallization and melting. The technique was applied to argon, tin and beryllium. Tin is modeled with the EAM potential, well reproducing the properties of BCC phase. Beryllium is modeled with the GEAM/MEAM potential.
2:00PM Q6.00002 The MD simulation on the micro-mechanism of micro-spallation of metal Pb under shock loading. JUN CHEN, MEIZHEN XIANG, Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, HAIHO HU, CAEP — We study the micro-mechanism of crystal and nano-crystal metal Pb under shock loading by using the molecular dynamics method. A wide range of shock intensity is conducted with the lowest one just above the threshold of solid spallation, while the highest one higher than the threshold of shock melting. The spallation mechanism is dominated by cavitation, i.e., nucleation, growth and coalescence of voids, as well as the interplay of cavitation and melting. Our results discovered that the grain boundary plays an important effect in the case of relieving melting, while it is smaller effect on the cases of conventional spallation and shock melting. The cavitation initiation forming first in form on the grain boundary, and they display mutual promotion: melting makes the void nucleation at smaller tensile stress; void growth speeds the melting. The spall strength dependence on the grain boundary, void and melting temperature is qualitatively discussed. Due to grain boundary effects, the spall strength of nano-crystalline Pb is less sensitive to shock intensity than single-crystalline Pb if cavitation occurs in solid state materials. If melting starts before cavitation, the spall strength of both nano-crystalline and single-crystalline Pb decreases dramatically as shock intensity increases.

2:15PM Q6.00003 Atomic models of plasticity of metals and alloys under dynamic loading. ALEXEY KUKSIN, ALEXEY YANILKIN, All-Russia Research Institute of Automatics, COMPUTATIONAL MATERIALS SCIENCE TEAM — The work presented is devoted to study the mechanisms and kinetics of plastic deformation of bcc and fcc metals and alloys under shock-wave loading (strain rates $10^4$ s$^{-1}$). To study the behavior of metals under conditions described the two scale approach is developed. It comprises molecular dynamics (MD) calculations of dislocation mobility and dislocations nucleation rate and continuum mechanics model with equations for description of elastoplastic deformation, kinetics and dynamics of dislocations. Dislocation velocities as functions of applied shear stress are calculated in Al, Cu, Fe, Mo from MD in a wide temperature range up to the melting point. Velocity-dependent drag coefficient is introduced to approximate the data obtained. The influence of Guinier-Preston (GP) zones on dislocation motion is analyzed. The results obtained are used to determine relaxation dependence of dynamic flow stress and the evolution of dislocations subsystem under shock loading. Data on the attenuation of the elastic precursor and rare surface velocity profiles calculated for Al in good agreement with the experiments. Simulation of the free surface velocity profiles during shock-wave loading of AlCu alloys is carried out.

2:30PM Q6.00004 Shock induced deformation twinning in tantalum MD simulations. MATTHEW SUGGIT, ANDREW HIGGINbotham, GABRIELE Mogni, JUSTIN WARK, University of Oxford, UK, EDUARDO BRINGA, Universidad Nacional de Cuyo, Mendoza, Argentina, PAUL ERHART, JAMES HREWLEK, BRUCE REMINGTON, LLNL, NIGEL PARK, AWE, Aldermaston, UK — Twinning is a potentially important deformation mechanism for shock compression of materials such as tantalum. We present large-scale molecular dynamics (MD) simulations of shock compression of tantalum employing an extended Finnis-Sinclair (EFS) potential. For shock loading along the [100] axis, the plastic deformation mechanism is demonstrated to be twinning using the Fourier transform of the atomic positions, and a new per atom structure factor (PASF) method. Using this method, the atoms can be accurately separated into each twin variant and the stress and strain calculated individually. Locally, the individual twins support a large strain anisotropy and deviatoric stress, which is globally reduced towards the hydrostatic. The mechanism of deformation twinning in the bcc structure is usually described by the successive displacement of (112) planes. In these simulations, the twinning mechanism is identified as the short range shuffling of alternate (112) planes after the large uniaxial compression due to the elastic precursor.

3:00PM Q6.00006 Molecular dynamics simulations of shock wave propagation in single crystal copper. ROMAIN PERRIOT, VASILY ZHAHKOVSKY, IVAN OLEYNIK, University of South Florida — Various regimes of shock wave propagation, including both plastic-split shock waves and single two-zone elastic-plastic shock waves, were studied by molecular dynamics (MD) simulations in single crystal copper oriented along the <100>, <110>, and <111> directions using both traditional piston-driven and the newly developed moving window MD techniques. The single two-zone elastic-plastic shock wave consists of the elastic zone followed by a plastic zone, where both elastic and plastic fronts move with the same speed, thus maintaining on average a constant separation. Although the properties of the leading elastic zone in both split-shock wave and single two-zone regimes are orientation-dependent, the thermodynamic properties of the plastic state are not once the steady-state regime is achieved in micrometer-thick films. The orientation-independent plastic Hugoniot obtained in our MD simulations agree with experimental observations of orientation-independent shock-wave propagation in single crystal copper [1].


Wednesday, July 10, 2013 1:45PM - 3:15PM – Session Q7 Energetic Materials and Postdeadline Grand Crescent - Evan Reed, Stanford University

1:45PM Q7.00001 Jetting Formation of Explosive Dispersal of Hybrid Particles. KUN XUE, State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing, 100081, China — The explosive dispersal of granular matter is characterized by persistent ballistic conical jets with billowing wakes. This particle clustering or jet structures influence but only their dynamic trajectories but also the particle-fluid mixing and subsequent energy release if the particles are reactive. The explosive dispersal of hybrid sand with a range of saturation were observed to exhibit a postoned jetting onset and a significantly finer and more uniformed jet structure with increasing saturation. In order to predict the particle jetting formation, we proposed an instability criterion involving the opposing forces of stabilizing inertial pressures and destabilizing viscous resistance. Thus a kinetic breakup model was established. The predicted instability onsets of expanding sand shells agreed reasonably well with the experimental observations. The incorporation of a modified granular compaction model taking into account the lubrication effect of interstitial fluids in hybrid sand enables the breakup model to quantitatively describe the dependence of jetting onset on the saturation. A close inspection of dynamic fragmentation of sand subject to explosive loadings via a multi-material hydrodynamic modeling revealed a multiple necking mechanism underlying the jetting formation opposed to the surface instability mechanisms, such as Rayleigh-Taylor (RT), Richtmyer-Meshkov instabilities (RM).

3:00PM Q6.00006 Molecular dynamics simulations of shock wave propagation in single crystal copper, ROMAIN PERRIOT, VASILY ZHAHKOVSKY, IVAN OLEYNIK, University of South Florida — Various regimes of shock wave propagation, including both plastic-split shock waves and single two-zone elastic-plastic shock waves, were studied by molecular dynamics (MD) simulations in single crystal copper oriented along the <100>, <110>, and <111> directions using both traditional piston-driven and the newly developed moving window MD techniques. The single two-zone elastic-plastic shock wave consists of the elastic zone followed by a plastic zone, where both elastic and plastic fronts move with the same speed, thus maintaining on average a constant separation. Although the properties of the leading elastic zone in both split-shock wave and single two-zone regimes are orientation-dependent, the thermodynamic properties of the plastic state are not once the steady-state regime is achieved in micrometer-thick films. The orientation-independent plastic Hugoniot obtained in our MD simulations agree with experimental observations of orientation-independent shock-wave propagation in single crystal copper [1].

2:00PM Q7.00002 Modeling anisotropic sensitivity in pentaerythritol tetranitrate using strain rate dependent reactive flow model1,2, KIHONG KIM2, LLNL & Seoul National University, LAURENCE E. FRIED, LLNL, JACK J. YOH, Seoul National University — Initiation of detonation in some high explosives has shown strong anisotropic sensitivity under mechanical impact. Preferred directions of crystal orientation on shock initiation have been experimentally observed in pentaerythritol tetranitrate (PETN), which resulted in dramatic difference in the detonation sensitivity upon shock compression in different directions. The ignition and growth model based on empirical observation on the pressure-dependent initiation of detonation has been widely used to date. Since the model is independent of direction of compression, it is impossible to address sensitivity associated with preferred crystal orientation for establishing the go/no-go criteria. In this paper, we have proposed a new reaction flow model that is consistent with available PETN experiments and atomistic calculations. A general tensor notation is utilized to fully address three-dimensional effect of the strain rate dependence to anisotropic detonation of PETN.

1K. Kim was supported by post-doctoral research fellowship from the National Research Foundation of Korea
2Visiting Research Fellow of LLNL & Post doctoral Fellow of Seoul National University

2:15PM Q7.00003 Quantum mechanical simulations of condensed-phase decomposition dynamics in molten RDX1, IGOR SCHWEIGERT, Naval Research Laboratory — A reaction model for condensed-phase decomposition of RDX under pressures up to several GPa is needed to support mesoscale simulations of the energetic material’s sensitivity to thermal and shock loading. A prerequisite to developing such a model is the identification of the chemical pathways that control the rate of the initial dissociation and the subsequent decomposition of molecular fragments. We use quantum mechanics based molecular dynamics simulations to follow the decomposition dynamics under high-pressure conditions and to identify the reaction mechanisms. This presentation will describe current applications to the liquid-phase decomposition of molten RDX.

3This work was supported by the Naval Research Laboratory, by the Office of Naval Research, and by the DOD High Performance Computing Modernization Program Software Application Institute for Multiscale Reactive Modeling of Insensitive Munitions

2:30PM Q7.00004 Time-Resolved K-shell Photoabsorption Edge Measurement in a Strongly Coupled Matter Driven by Laser-converted Radiation, YANG ZHAO, Research Center of Laser Fusion, China Academy of Engineering Physics, Miyun County 102208, China. A coupling force between undulations of lasing light and the photoabsorption edge of material leads to the photoabsorption of such undulations. The laser undulations are usually in the order of 1019 W/m2. It is very difficult to detect the photoabsorption edge under such powerful undulations. We used a novel technique to produce and record such photoabsorption edges. This technique has successfully applied in many areas such as high temperature, high pressure, and high magnetic field regions. We conducted a series of experiments under a pressure of 3 GPa and a magnetic field of 10 T. The photoabsorption edge was detected in the range of ~23 kcal/mol.

2:45PM Q7.00005 Enhanced sensitivity of explosives in the Condensed Phase: 2,4,6-trinitrotoluene as a model, YEHUDA ZEIRI, NRCN and Ben-Gurion University, Beer-Sheva, Israel, DAVID FURMAN, FAINA DUBNIKOVA, NAOMI ROM, BARAK HIRSHBERG, Hebrew University, Jerusalem, Israel, SERGEY V. ZYBIN, WILLIAM A. GODDARD III, Caltech, CA, USA, RONNIE KOSLOFF, Hebrew University, Jerusalem, Israel — This study is based on the results of Molecular Dynamics (MD) employing a reactive force field (ReaxFF) and electronic structure (DFT) calculations of 2,4,6-trinitrotoluene (TNT) decomposition and high temperatures and pressures. The sensitivity to decomposition shows a marked increase for the condensed phase as compared with single molecule. The simulations suggest that bimolecular processes dominate the initial stages of decomposition. The DFT calculations used to explore the role of bimolecular pathways. These pathways are responsible to the ~23 kcal/mol reduction in the barrier height that lead to the enhanced sensitivity. These pathways involve (1) an H atom transfer between two neighboring TNT molecules in from the aromatic ring of one to one of the nitro groups of the other. The loss of the H atom promotes breaking the adjacent C-NO2, and (2) the H atom transfer to the NO2 leads subsequently to the formation of HONO and NO products. The thermal decomposition process was followed using the MD simulations for 400 ps to reach the final stable decomposition products. In addition to stable gas products, we obtained carbon clusters formed by the agglomeration of aromatic rings. The TNT decomposition mechanism is compared to that of other explosives.

3:00PM Q7.00006 Measurements of Shaped Charge Jet Velocity, HONGFA HUANG, Schlumberger Perforating Research — Penetration depth is an important requirement in oil/gas well perforating jobs. The depth determines how far the wellbore will directly communicate with reservoir fluids. Deep perforation charges are widely used in oilfield industry and most of those are powder metal liner charge for no carrot-like slug left as solid liner does. Comprehensive measurements for the powder metal liner shaped charge jet characteristics, namely, the jet density and velocity, are needed to predict the shaped charge performance and to plan the perforating job. This paper focuses on an experimental work of jet velocity measurements. A medium size of powder metal liner charges (27 grams HMx) is used in the tests. The powder jet shoots through a stack of limestone blocks with shorting switch set in between. Half inch air-gap between two blocks is design to provide space for jet traveling in air to record free fly velocity, meanwhile the jet penetration velocity in the limestone is measured. Aluminum foil switches are used to record the jet Time of Arrival (TOA). The charged switch shorted by the metal jet when it arrives. The shorting signal is recorded. The two velocities can be used to estimate the jet penetration effectiveness. A series of TOA tests show that jet velocity along its length linearly decreases from jet tip to tail until the stagnation points referring to which jet material moves in opposite direction.

Wednesday, July 10, 2013 3:30PM - 5:30PM – Session R1 ME.3 Inelastic Deformation, Fracture, and Spall VII Grand Ballroom I - James Stalken, Lawrence Livermore National Laboratory
expected to be suppressed. We make comparisons with similar data obtained from experiments conducted on roll-textured plate where the contribution of twinning to initial deformation is the observed precursor decay with respect to the relative roles of twinning and dislocation mediated slip in the overall material mechanical response. We will discuss the observed precursor decay with respect to the relative roles of twinning and dislocation mediated slip in the overall material mechanical response. We will make comparisons with similar data obtained from experiments conducted on roll-textured plate where the contribution of twinning to initial deformation is expected to be suppressed.

WILLIAM R. BLUMENTHAL, GEORGE (RUSTY) T. GRAY, III, Los Alamos National Laboratory — We have performed a number of plate impact experiments controlled by the extent of brittle particles that acted as nucleation sites for damage during tensile failure. Despite large differences in the HEL, the spall behavior for Al 5083 made by both processing techniques was hardening. Materials processed by ECAE have a highly refined grain structure with little texturing and a large degree of plastic deformation, whereas rolled strain-hardenable aluminum alloy used for armor plating in military transport vehicles, thus requiring the highest achievable spall strength. The spall strength aluminum alloy 5083 (Al 5083) are compared for plates fabricated using equi-channel angular extrusion (ECAE) versus rolling. Al 5083 is a light-weight and technologically important material.

SUVEEN MATHAUDHU, Army Research Office, LASZLO KECSKES, Army Research Laboratory — The spall strength and Hugoniot Elastic Limit (HEL) of Angular Extrusion and Rolling.

3:30PM R1.00001 Elastic Precursor Decay in S-200F Beryllium. CHRIS D. ADAMS, WILLIAM W. ANDERSON, WILLIAM R. BLUMENTHAL, GEORGE (RUSTY) T. GRAY, III, Los Alamos National Laboratory — We have performed a number of plate impact experiments on vacuum hot-pressed (VHP) S-200F Be at shock stresses between 2.1 and 23 GPa to gain insight into the dynamic strength and damage behavior of this material. In this discussion we will focus on our observations of dynamic strength represented by the Hugoniot Elastic Limit (HEL) determined from the amplitude of the elastic precursor wave observed in VISAR wave profiles collected at the rear surface of the target for experiments conducted in transmission geometry. We observe monotonic decay in precursor amplitude with run distance for sample thicknesses between 4 and 8 mm. We will discuss the observed precursor decay with respect to the relative roles of twinning and dislocation mediated slip in the overall material mechanical response. We will compare our observations with similar data obtained from experiments on roll-textured plate where the contribution of twinning to initial deformation is expected to be suppressed.


3:45PM R1.00002 Characterization of shocked beryllium. CARL CADY, ERIC BROWN, GEORGE GRAY, CHRIS ADAMS, LAWRENCE HULL, THOMAS WYNN, MICHAEL PRIME, JAMES COLEY, CURT BRONKHORST, FRANK ADDESSIO, Los Alamos National Laboratory — Explosively driven arrested beryllium experiments were performed with post mortem characterization to evaluate the microstructure and failure behaviors. The test samples were encapsulated in an aluminum assembly that was large relative to the sample, and the assembly features both axial and radial momentum traps. The sample carrier was inserted from the explosively loaded end and has features to lock the carrier to the surrounding cylinder using the induced plastic flow. Calculations with Lagrangian codes showed that the tensile stresses experienced by the Be sample were below the spall stress. Metallographic characterization of the arrested Be showed radial cracks present in the samples may have been caused by bending moments. Fractography showed the fractures propagated from the side of the sample closest to the explosives, the side with the highest tensile stress. There was evidence that the fractures may have propagated from the circumferential crack outward and downward radially. The EBSD results were the most informative of the characterization techniques used. EBSD provides information regarding texture, residual strain, and twinning. There was clear evidence of grain rotation as evidenced by the pole figures, the inverse pole figures and the Kernel Average Mismatch figures.

4:00PM R1.00003 ABSTRACT HAS BEEN MOVED TO M1.00107 –

4:15PM R1.00004 Calibrating a Shear-failure model using punch specimens in the SHPB apparatus. ZEV LOVINGER, YEHEZKEL ASHUACH, RAFAEL — We are using a punch specimen on the split Hopkinson pressure bar (SHPB) apparatus to calibrate a shear failure model for two Aluminum alloys. The tested specimen is a thin disc which is placed between punch and anvil adapters. We use 2D simulations of the entire SHPB set-up and compare the experimental strain-gauge measurements to our numerical gauges in the model. The straight forward procedure we developed consists of two stages: first, we fit a strength model based on the standard Hopkinson analysis and validate the model through simulations of the SHPB test, comparing the strain-gauge signals. At the second stage we use the validated strength model and calibrate the shear failure model parameters by fitting the fall-time of the transmitted signal. The fall time is found to be very sensitive to the failure parameters. Finally, we conducted FSP penetration tests to validate the failure model and found good comparison with our simulations.

4:30PM R1.00005 Spall Properties of Aluminum 5083 Plate Fabricated using Equi-Channel Angular Extrusion and Rolling. RICKY WHELCHEL, NARESH THADHANI, THOMAS SANDERS, Georgia Institute of Technology, SUVEEN MATHAUDHU, Army Research Office, LASZLO KECSKES, Army Research Laboratory — The spall strength and Hugoniot Elastic Limit (HEL) of aluminum alloy 5083 (Al 5083) are compared for plates fabricated using equi-channel angular extrusion (ECAE) versus rolling. Al 5083 is a light-weight and strain-hardenable aluminum alloy used for armor plating in military transport vehicles, thus requiring the highest achievable spall strength. The spall strength of strain-hardenable alloys is a function of the grain structure and volume fraction of secondary phases, such as brittle inclusions, in addition to the extent of hardening. Materials processed by ECAE have a highly refined grain structure with little texturing and a large degree of plastic deformation, whereas rolled plates have a textured grain structure that aligns along the rolling direction. The spall behavior of Al 5083 for both forms was measured using plate impact gas gun experiments combined with rare free surface velocity measurements employing VISAR. The spall strength varied with impact orientation for the rolled plate but remained uniform for the ECAE material. Despite large differences in the HEL, the spall behavior for Al 5083 was made by both processing techniques was controlled by the extent of brittle particles that acted as nucleation sites for damage during tensile failure.

4:45PM R1.00006 The shock and spall response of AA 7010-T7651. PAUL HAZELL, The University of New South Wales, GARETH APPLEBY-THOMAS, DAVID WOOD, JONATHAN PAINTER, Cranfield University — Aluminium alloys are used extensively in armour. Their use as armour materials is primarily due to their relatively low densities and their high strength characteristics. The aerospace-grade 7000-series alloy Al7010-T7651 is one possible contender for armour. In this study a series of plate-impact experiments were undertaken to investigate the behaviour of this alloy under shock. Mangani stress gauges and a heterodyne velocimeter system were used to interrogate both strength and dynamic tensile failure (spall) respectively; with microscopic analysis of recovered samples providing insight into the development of failure in the material.

5:00PM R1.00007 Effect of Dynamic Loading Rate on the Uniaxial Dynamic Tensile Response in Commercially Pure 1050 Aluminum. NATHANIEL SANCHEZ, DARCIE DENNIS-KOLLER, Los Alamos National Laboratory, DAVID FIELD, Washington State University — A series of plate impact experiments were conducted to investigate the effect of dynamic loading rate on the uniaxial dynamic tensile response of commercially pure 1050 aluminum. The loading rate (kinetic effect) was varied by altering the shock-wave shape, while the total defect density loaded in dynamic tension was held constant (spatial effect). The maximum tensile stress magnitude was held constant for all experiments in order to solely examine the effects of dynamic loading rate. Samples were soft recovered and analyzed via Electron Backscatter Diffraction (EBSD) to correlate damage to microstructural features. An optical velocimeter (VISAR) trace from the free surface was utilized to correlate the effects of damage growth rate observed through EBSD to changes in free surface velocity pull back rate. Results indicate as the dynamic tensile evolution rate was increased, a transition occurs from slow damage mechanisms of individual void nucleation and growth, to a fast mechanism of lattice curvature resulting in no observable macroscopic damage. These results suggest damage models must account for wave evolution in order to provide a robust predictive capability.
5:15PM R1.00008 Study on the characteristics of dynamic damage in ultrapure Aluminum with 2D and 3D method, MEILAN QI1, BIXIONG BIE, School of Science, Wuhan University of Technology, CHANGMING HU, HONGLIANG HE, National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, CAEP, XIAOXIA RAN, DUAN PAN, School of Science, Wuhan University of Technology, SHENGNIAN LUO, The Peac Institute of Multiscale Sciences, Sichuan University — Based on the metallographic analysis, electron back scattering diffraction and 3D tomography with synchrotron x-ray method, the characteristics and laws of damage distribution in ultrapure aluminum with different degree under shock loading are characterized and analyzed. Some microscopic characteristics of damages are worthy of attention. Under the low-velocity impact, inhomogeneous void will grow in isolation, and the space distribution of voids is uneven in the area with same tensile stress, which is related to the microstructure of the material. Under higher-velocity impact, the voids will grow bigger and connect each other, which lead to the concentrated area of damage. The space distribution of voids and the connecting form of two voids can be found clearly from the 3D analysis result. Moreover, the result of electron back scattering diffraction shows that the emitted dislocation will appear during the growth process of voids, which accelerates the growth of voids and make the voids easy to coalesce each other.

1 mail address: 410-B3163B, HP8SynChX-ray, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA

Wednesday, July 10, 2013 3:30PM - 5:30PM  
Session R2 DR Dynamic Response of Materials  
Grand Ballroom II - Yogi Gupta, Washington State University, John Sarro, Los Alamos National Laboratory

3:00PM R2.00001 Dynamic Experiments using IMPULSE at the Advanced Photon Source, BRIAN JENSEN, Los Alamos National Laboratory — The ability to examine the dynamic response of materials at extreme conditions requires diagnostics that can provide new tools to study shock phenomena. Several advances in synchrotron sources and diagnostics coupled to dynamic loading platforms are transforming the dynamic compression field to allow for such investigations. In the current work, recent experimental efforts on the IMPULSE (IMPact System for ULtrafast Synchrotron Experiments) capability at the Advanced Photon Source (Argonne, IL) will be highlighted to describe the development of the capability and its use to examine phenomena including jet-formation in metals, compaction, crack formation and propagation, and material strength and failure. These experimental results have relied in part on: 1) the development of a robust optically multiplexed intensified detector configuration to obtain the first shock movies and 2) gun system improvements to better synchronize the impact event with the 60-ps width X-ray bunch. The IMPULSE capability is expected to continue to reveal novel phenomena for materials subjected to high strain rate loading while developing the required knowledge base to ensure success for future facilities including the Dynamic Compression Sector at the Advanced Photon Source and LANL’s MaRIE.

3:50PM R2.00002 X-ray Diffraction on Shocked Solids: Past Results and Future Prospects at the Dynamic Compression Sector, STEFAN TURNÉAURE, Wash. State Univ. — Real-time X-ray diffraction measurements in shocked solids represent an important development for understanding the response of shocked solids at the lattice and microscopic levels. Two examples of recent X-ray diffraction work on shock compressed single crystals will be reviewed. First, insight into shocked crystal microstructure was obtained through analysis of X-ray diffraction peak broadening caused by shock-induced microstructural heterogeneities. Second, macroscopic strength of single crystals shock compressed above their yield stress with 3-femtosecond temporal resolution was determined from average longitudinal lattice strain (determined from X-ray diffraction) and macroscopic longitudinal stress (determined from continuum methods). The use of X-rays as a probe of the shocked state will be greatly enhanced by the Dynamic Compression Sector (DCS), currently under development at the Advanced Photon Source (APS). The DCS, a user facility, will be dedicated to understanding dynamically compressed condensed matter using X-ray scattering/diffraction and X-ray imaging measurements. X-ray measurement timescales will vary from about 100 ps to over a µs and multi-frame capabilities will allow time-dependent changes to be monitored. An overview of the planned X-ray beam characteristics at DCS will be used to show simulations of various material phenomena of interest in dynamic compression research. Simulation results will also be compared to single pulse X-ray diffraction measurements at the APS on ambient samples. Work supported by DOE/NNSA, and carried out in collaboration with Y. M. Gupta.

4:10PM R2.00003 Observation of ultrafast dynamic compression at the lattice-level; experimental capabilities and early science at the Linac Coherent Light Source, HAE JA LEE, SLAC National Accelerator Laboratory — An in-depth understanding of the stress-strain behavior of materials during ultrafast dynamic compression requires experiments that offer in-situ observation of the lattice at the pertinent temporal and spatial scales. To date, the lattice response under extreme strain-rate conditions (>108 s-1) has been inferred predominantly from continuum-level measurements and multi-million atom molecular dynamics simulations. Several time-resolved x-ray diffraction experiments have captured important information on plasticity kinetics, while limited to nanosecond timescales due to the lack of high brilliance ultrafast x-ray sources. Here we present new experimental capabilities at the Linac Coherent Light Source (LCLS) combining ultrafast laser-shocks and sequential femtosecond x-ray diffraction. The high spectral brightness (~ 1012 photons per pulse, ∆E/E = 0.2%) and subpicosecond temporal resolution (<100 fs pulsewidth) of the LCLS x-ray free electron laser allow investigations that link simulations and experiments at the fundamental temporal and spatial scales for the first time, thus enabling validation of plasticity models at these extreme strain rates. We describe early pump-probe experiments at LCLS that offer insights to the transient lattice states and compare with predictions from large-scale molecular dynamics simulations. A movie of the lattice undergoing rapid shock-compression, composed by a series of single femtosecond x-ray snapshots, demonstrates the transient behavior while successfully decoupling the elastic and plastic response in a polycrystalline material. We discuss future directions at LCLS can offer to the material science community, ultimately leading to a predictive understanding and control of the material response during ultrafast dynamic compression.

4:30PM R2.00004 In-situ probing of Low Density Porous Materials, JAMES HARRELIKAJ, LLNL — The shock response of porous materials is of interest in High Energy Density Physics because the PdV heating from void closure allows off principle Hugoniot states for modeling many astrophysical processes. While continuum models exists of shockwave propagation in foams the relevant physical phenomena spans three different length scales: the micro-length scale defined by the pore size and length between solid structures in the foam (10 to 1000nm), the shock front thickness which determines material and energy flow (0.1 to 100nm), and the hydrodynamic length scale associated with the expanding spherical wave (>10 μm), all of which impact the shock response of the low density foam. With the advent of new HED experimental facilities for generating shockwaves at x-ray light sources this gives new tools for performing pump probe experiments to understand the microstructural response of low density materials. Currently, we have used x-ray radiography to make Hugoniot EOS measurements of the shock compressed low density SiO2 and Carbon based foams. We will show recent result of measurements of experiments conducted on the Omega laser facility and discuss imaging shockwaves in low density foams on the soon to be commissioned DCS end station at APS and the MEC end station at LCLS. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

4:50PM R2.00005 Panel Discussion —
3:30PM R3.00001 From microns to millimeters: New Diamond Cells for Multi-Megabar pressures and for Neutron Diffraction, REINHARD BOEHLER, MUHTAR AHART, MALCOLM GUTHRIE, Geophysical Laboratory, Washington, DC, USA, JAMIE MOLAISON, CHRISTOPHER TULK, Neutron Sciences Directorate, ORNL, Oak Ridge, TN, USA — We developed new diamond cells for two extreme applications. One cell was designed to routinely study hydrogen above 2 Megabar (200 GPa) [2] by adopting the principle of deflecting plates reported earlier [1]. Neutron defraction requires millimeter-sized samples even for the very high neutron fluxes available at the Oak ridge National Laboratory. We develop a new diamond cell capable of routinely reaching pressures of 80 GPa with culets of 1.5 mm. The diamonds were of only 4 mm diameter with conical design [3] using strongly supported seats made of polycrystalline diamond. We present new, high-quality data for D$_2$O showing signs of symmetrisation in ice [4]. Tests using very large CVD diamonds are in progress.


3:45PM R3.00002 A New Way of Generating Load at Cryogenic Temperatures for Neutron Studies, MATTHEW JACOBSEN, CHRISTOPHER RIDELEY, School of Engineering and Centre for Science at Extreme Conditions, University of Edinburgh, United Kingdom, OLEG KIRICHUK, PASCAL MANUEL, ISIS, Rutherford Appleton Laboratory, United Kingdom, PAUL ATTFIELD, School of Chemistry and Centre for Science at Extreme Conditions, University of Edinburgh, United Kingdom, KONSTANTIN KAMENEV, School of Engineering and Centre for Science at Extreme Conditions, University of Edinburgh, United Kingdom — Pressure generation at cryogenic temperatures presents a problem for a wide array of experimental techniques, particularly for neutron studies due to the volume of sample required [1]. This challenge has been previously tackled by using a modified Bridgman-seal in a Paris-Edinburgh cell [2]. We present a novel design of a pressure cell in which load is generated by a bellows driven by helium gas which ensures leak-free operation of the device. The bellows is custom-designed to generate the load of 80 kN at the maximum operational gas pressure of 350 bar. For opposed anvils with 3 mm diameter working surface, for example, this load converts into an average pressure of 11 GPa across the culets. The cell has four large windows for the scattered beam and the setup allows control of pressure in a wide (P,T) range in which helium is in gas or liquid state. The cell has been used at the WISH beamline of the ISIS Pulsed Neutron Source with sapphire anvils. The device will be presented in detail, along with pressure loading curves and initial experimental data.


4:00PM R3.00003 X-ray imaging in the large volume Paris-Edinburgh press, JEAN-PHILIPPE PERRILLAT, Laboratoire de Géologie de Lyon, UMR5276, Université Claude Bernard Lyon1, CNRS and ENS Lyon, France — Synchrotron X-ray tomography is a non-destructive 3D imaging/microanalysis technique selective to a wide range of properties such as density, chemical composition, chemical states, structure, and crystallographic perfection; with extremely high sensitivity and spatial resolution. We describe a new device, based on the V7 Paris-Edinburgh press, to extend this technique to high-pressure high-temperature conditions. It consists of two opposed conical anvils to pressurize the sample encased in an X-ray transparent boron epoxy gasket. Both anvils can rotate, with no limitation in the rotating angles, through two sets of gear reducer and thrust bearings located at the end of each anvil. The accurate and simultaneous rotation of the top and bottom anvils is monitored by stepper motors and encoders. This enables the collection of data at small angular steps over 180° rotation required for a complete 3D tomographic reconstruction. The potentials of this new equipment will be illustrated on two examples: (1) the determination of the volumetric properties of materials by absorption contrast tomography, and (2) the characterisation of ill-ordered materials under HP-HT by X-ray diffraction tomography.

4:30PM R3.00004 Limitations and possibilities of AC calorimetry in diamond anvil cells, ZACHARY GEBALLE, UC Berkeley, GILBERT COLINS, LLNL, RAYMOND JEANLOZ, UC Berkeley — Dynamic laser heating or internal resistive heating could allow for the determination of calorimetric properties of samples that are held statically at high pressure. However, the highly non-adiabatic environment of high-pressure cells presents several challenges. Here, we quantify the errors in AC calorimetry measurements using laser heating or internal resistive heating inside diamond anvil cells, summarize the equipment requirements of supplying sufficient power modulated at a high enough frequency to measure specific heats and latent heats of phase transitions, and propose two new experiments in internally-heated diamond anvil cells: an absolute measurement of specific heat (with ∼10% uncertainty) of non-magnetic metals using resistive heating at ∼10 MHz, and a relative measurement to detect changes in either the specific heat of metals or in the effusively (the product of specific heat, density and thermal conductivity) of an insulator.

4:45PM R3.00005 High pressure modifications of the liquid structure of the light alkaline metals, GASTON GARBARINO, European Synchrotron Radiation Facility (ESRF); Grenoble; France, GUNNAR WECK, Département de Physique Théorique et Appliquée;CEA/DAM Ile de France; France, PIERRE BOUVIER, Lab. des Matériaux et du Génie Physique LMGEP (CNRS/Grenoble INP); Grenoble; France, MOHAMED MEZOUAR, European Synchrotron Radiation Facility (ESRF); Grenoble; France — The alkali group elements are considered as textbook examples of free-electron metals because of the single s electron in the valence band. However, when these metals are subjected to compression they exhibit unexpected complexity suggesting extraordinary liquid states at extreme conditions. The analysis of the liquid structures of the light alkali metals has not been completed because of the lack of experimental data. Only X ray diffraction (XRD) data at room pressure are available. The major difficulty with liquid diffraction at high pressure is the large scattering background signal generated by the diamond anvil cell giving a signal over background ratio of around only 1 to 5 per cent. All these points explain the lack of experimental data of liquid alkali metals at high pressure. We performed the first quantitative measurements of the liquid structure factor of light alkali metals up to 100 GPa using XRD. We explored the P-T diagram in order to obtain quantitative structure factor, radial-distribution function and density of alkali metals up to 100 GPa. We confirmed the existence of a different liquid structure at the minimum of the melting curve compared with the one at room pressure.
5:00PM R3.00006 Kinetics of Phase Transitions in Simple Materials using dynamic-DAC¹.
JING-YIN CHEN, Lawrence Livermore National Laboratory — The pressure-induced phase transition is often limited by diffusion and occurs at the intermediate time-scale (μs to ns) of shock wave and static DAC high pressure experiments, which can be obtained precisely and in controlled ways using dynamic-DAC. Coupling it with time-resolved optical spectroscopy and time-resolved synchrotron x-ray diffraction, we have recently studied high-pressure kinetics of phase transitions in a variety of materials including Bi, Ga, Fe, H₂O, and methane hydrates. In this presentation, we will first describe the experimental methods and then present the results of (i) solidification of H₂O and Ga, (ii) phase transitions in Bi and Fe, and methane hydrates, and (iii) solid-state reactions in methane hydrates. As such, we will demonstrate the significance of obtaining the time-resolved structural information to understand the phase meta/stability, transition mechanisms, and diffusion-controlled crystal growth and interfacial reactions in solids.

In collaboration with Hyunchae Cynn, Lawrence Livermore National Laboratory; Choong-Shik Yoo, Department of Chemistry and Institute for Shock Physics, Washington State University; and William Evans, Lawrence Livermore National Laboratory.

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Wednesday, July 10, 2013 3:30PM - 5:30PM —
Session R4 NM.3 Novel Properties II Vashon - Daniel Eakins, Imperial College London

3:30PM R4.00001 Recent Studies in Electrical Transport Properties at Extreme Pressures.
TAKAHIRO MATSUOKA, Center for Quantum Science and Technology under Extreme Conditions — High pressure plays important roles in expanding our understanding of materials. Electrical transport properties significantly change as pressure brings atoms and molecules close together. For example, O₂, which is insulator under ambient pressure, becomes metallic and even a superconductor under high pressures exceeding 95 GPa [1, 2]. Recently, conductive H₂ has been reported at near around 220 GPa and room temperature [3]. On the other hand, Li and Na have been found to become a semiconductor and an insulator in dense conditions that ion core-valence overlap becomes significant [4,5]. The number of elemental superconductors is increasing with the development of high-pressure techniques. Currently 22 of 52 elemental superconductors are known to superconduct only at high pressures. In this talk we discuss very recent experiments that revealed re-entrant metallic and superconducting phase of Li at above 100 GPa. In addition, the simultaneous measurement system of X-ray diffraction, Raman scattering and electrical resistance in BL10XU/SPring-8 is presented. In order to study electrical properties, including superconductivity in detail, and reveal underlying physics, it is very important to observe crystal structures and electrical resistance simultaneously at high pressures. Li becomes a semiconductor at above 80 GPa accompanied with structural transformation [4]. Recently we have observed experimentally that Li reverts to a metal accompanied with Tc above 10 K. High electrical resistivity value and abrupt appearance of superconductivity may indicate that Li in O24 is a poor metal with atypical electronic states. The present study found a phase diagram, a semiconductor phase between superconducting phases, not previously observed for any materials.


4:00PM R4.00002 Strain Rate Behavior of HTPB-Based Magnetorheological Materials¹.
CHAD STOLTZ, KENNETH SEMINUK, VASANT JOSHI, Naval Surface Warfare Center, Indian Head Division — It is of particular interest to determine whether the mechanical properties of binder systems can be manipulated by adding ferrous or Magnetostriective particulates. Strain rate response of two HTPB/Fe (Hydroxyl-terminated Polybutadiene/ Iron) compositions under electromagnetic fields has been investigated using a Split Hopkinson Pressure bar arrangement equipped with aluminum bars. Two HTPB/Fe compositions were developed, the first without plasticizer and the second containing plasticizer. Samples were tested with and without the application of a 0.01 Tesla magnetic field coil. Strain gauge data taken from the Split Hopkinson Pressure bar has been used to determine what structural properties were changed by inducing a mild electromagnetic field onto each sample. The data reduction method to obtain stress-strain plots included dispersion corrections for deciphering minute changes due to compositional alterations. Data collected from the Split Hopkinson Pressure bar indicate changes in the Mechanical Stress-Strain curves suggest that the impedance of a binder system can be altered by means of a magnetic field.

¹We acknowledge the Defense Threat Reduction Agency for funding.

4:15PM R4.00003 Brazilian Disc Experiments on a Cold Spray Material.
C.H. BRAITHWAITE, Fracture and Shock Physics, SMF Group, Department of Physics, Cavendish Laboratory, J J Thomson, Avenue, Cambridge CB3 0HE, UK, B. AYDELOTTE, Georgia Institute of Technology School of Materials Science and Engineering, 771 Ferst Drive, J. Erskine Love Building, Atlanta, GA 30332-0245 USA, A.P. JARDINE, Fracture and Shock Physics, SMF Group, Department of Physics, Cavendish Laboratory, J J Thomson, Avenue, Cambridge CB3 0HE, UK — Characterisation of novel materials presents a number of unique difficulties to the experimenter, however these are problems which must be overcome in order to effectively utilise such materials in systems level applications. A series of experiments were performed to probe the tensile behaviour of a two cold sprayed composite materials containing a mixture of nickel, aluminium, tungsten and zirconium. Data were acquired at two different strain rates and collected using high speed photography, strain gauges, force-extension measurements and digital image correlation techniques. Comparisons were made with modelling on representative microstructural elements in the CTH code.

4:30PM R4.00004 Polycrystalline solids under nonhydrostatic compression: Determination of strength from x-ray diffraction data.
ANIL SINGH, Retired — A polycrystalline sample compressed in a diamond anvil cell (DAC) without any pressure transmitting medium develops a stress state at the center of the sample that is axially symmetric about the load axis. The axial stress component is larger than the radial component and the difference between the two is taken as a measure of compressive strength of the sample material at a confining pressure that equals the mean normal stress. The diffraction data taken from a sample under such a stress sate contain a range of information that is absent in the hydrostatic pressure data. A proper analysis of the data using the lattice strain theory yields compressive strength. The data taken with the radial diffraction geometry wherein the incident x-ray beam is perpendicular to the load axis of the DAC gives reliable estimates of strength. The diffraction data obtained with the conventional geometry wherein the incident x-ray beam passes parallel to the DAC axis are not suitable for a full range of analysis. However, reliable estimates of the strength can be obtained by combining the measured pressure-volume data under nonhydrostatic compression and the hydrostat derived from an independent source. The broadening of diffraction lines under nonhydrostatic compression has been also used to estimate the strength of crystalline solids. The effect of elasto-plastic deformation on the strength estimates will be discussed.

5:00PM R4.00005 ABSTRACT WITHDRAWN
5:15PM R4.00006 Response to Stress in Molecular Loops probed by Raman Spectroscopy. M. PENA-ALVAREZ, M. TARAVILLO, E. DEL CORRO, V.G. BAONZA, MALTA, Univ. Complutense of Madrid, Spain, M. KERTESZ, Georgetown Univ. Washington, USA, S. YAMAGO, Kyoto Univ. Japan, P. MAYORGA, J.T. LOPEZ-NAVARrete, J. CASADO, Univ. Malaga, Spain — CycloParaPhenylene (CPPs) are cyclic molecules formed by para-substituted benzenes. They are in the spot-light of chemistry because, in addition to their simple hoop-shaped π-conjugated structure, CPPs are thought of as building blocks for the controlled synthesis of carbon nanotubes (CNTs). Although they were firstly synthesized in 2008, their physico-chemical behavior is still poorly known, despite the interest in their optical properties, reactivity and their use as host agents in supramolecular chemistry. Studies about their possible analogies/differences with CNTs and other sp²-carbon structures are still lacking. Pressure-dependent Raman experiments provide key information about all the above properties, so here we present a Raman study on CPPs ranging from [6]CPP to [12]CPP. The pressure-induced changes in their vibrational spectra are analyzed in order to check whether pressure induces conformational changes and how these compare to those previously reported in their linear oligophenylene analogs. To explore their ability to form host-guest complexes with other carbon species, CPP-fullerene mixtures subjected to stress and their recovered samples are studied, concluding that the complex C_{60}@[10]CPP has been formed.

Wednesday, July 10, 2013 3:30PM - 5:30PM — Session R5 EM.1 Detonation II Cascade I - Carlos Chiquete, Los Alamos National Laboratory

3:30PM R5.00001 Experimental Measurement of the Scaling of the Diameter- and Thickness-Effect Curves for Ideal, Insensitive, and Non-Ideal Explosives. SCOTT JACKSON, MARK SHORT, Los Alamos National Laboratory — Numerous two-dimensional high-explosive slab rate sticks were fielded for explosives that exhibit ideal (PBX 9501), slightly non-ideal (PBX 9502), and highly non-ideal (ANFO) detonation. Detonation velocity versus slab thickness t (thickness-effect curves) are compared to previous diameter-effect measurements obtained by varying the diameter d of cylindrical rate sticks. The scale factors d/t necessary to overlay the diameter- and thickness-effect curves were computed for each explosive formulation. We observe that the scale factor varies with detonation velocity (or level of detonation “ideality”). The measured scale factors range from 1.89–2.20, 1.41–1.87, and 1.79–1.05 for PBX 9501, PBX 9502, and ANFO formulations, respectively, as detonation velocity varies from the (near failure) critical velocity to the Chapman-Jouguet velocity. These results support our previous theoretical prediction that the scale factor relating the diameter- and thickness-effect curves will increasingly deviate from two as the detonation structure becomes increasingly non-ideal.

3:45PM R5.00002 Critical detonation thickness in vapor-deposited hexanitroazobenzene (HNAB) films with different preparation conditions. ALEXANDER S. TAPPAN, ROBERT KNEEPER, MICHAEL P. MARQUEZ, J. PATRICK BALL, JILL C. MILLER, Sandia National Laboratories — At Sandia National Laboratories, we have coined the term “microenergetics” to describe sub-millimeter energetic material studies aimed at gaining knowledge of combustion and detonation behavior at the mesoscale. Films of the high explosive hexanitroazobenzene (HNAB) have been deposited through physical vapor deposition. HNAB deposits in an amorphous state that crystallizes over time and modest heating accelerates this crystallization. HNAB films were prepared under different crystallization temperatures, and characterized with surface profilometry and scanning electron microscopy. The critical detonation thickness for HNAB at different crystallization conditions was determined in a configuration where charge width was large compared to film thickness, and thus side losses did not play a role in detonation propagation. The results of these experiments will be discussed in the context of small sample geometry, deposited film morphology, crystal structure, and density.

4:00PM R5.00003 Converging shocks for DSD modelling. CHRISTOPHE MATIGNON¹, CEA, DAM, DIF, F-91297 Arpajon — Modelling of pyrotechnic systems requires both, a good understanding and precise prediction capabilities of the dynamics of detonation. When using insensitive high explosives IHE (such as TATB-based explosives) the interaction of the detonation front with the confinement can lead to very different detonation velocities. One of the most powerful engineering tools used to model this behaviour is the Detonation Shock Dynamics (DSD). In the DSD assumption, the detonation front propagates at a normal shock velocity (Dn) which depends only on its local curvature (κ). For divergent detonations, the DSD limit is very well established both experimentally and theoretically and one can easily propose a model (which obeys the 1D quasi-steady weakly curved detonation theory) to reproduce this behavior. We propose to extend the DSD theory to slightly convergent detonation fronts and to validate it against experimental data. Two series of experiments were carried out. The first series was designed to collect precise information regarding converging detonation. Usually, in such configurations, the detonation is non steady, making precise and simultaneous measurements of velocity and curvature difficult to achieve. The originality of the proposed setup is to drive a self similar convergent detonation at constant speed in an IHE rod by an external explosive tube of greater detonation velocity (allowing an accurate recording of both velocity and curvature). A wide range EOS/reaction rate model (inspired from previous works of Wescott et al.,) was then calibrated to reproduce both the strong shock initiation and the newly extended (D−κ) law. This model can be used to perform either direct numerical simulation (DNS) on fine resolved mesh grid, or its reduced PZR model (DSD based) on a much coarser grid. This model was then successfully validated against the second series of experiments involving a detonation propagating around an obstacle and exhibiting a non steady converging front while passing the obstacle. Discussions will be focussed on the uniqueness of the (D−κ) law on the converging branch (κ < 0) and the ability of DSD to reproduce accelerating detonation fronts through comparisons between DSD and DNS calculations with experimental data.

¹Co-authors: R. Sorin, O. Bozier, N. Desbiens, V. Dubois, CEA, DAM, DIF, F-91297 Arpajon

4:30PM R5.00004 Modelling an IHE Experiment with a Suite of DSD Models. ALEXANDER HODGSON, AWE, Aldermaston — At the 2011 APS conference, Terrones, Burkett and Morris published an experiment primarily designed to allow examination of the propagation of a detonation front in a 3-dimensional charge of PBX9502 insensitive high explosive. The charge is confined by a cylindrical steel shell, has an elliptical tin liner, and is line-initiated along its length. The detonation wave must propagate around the inner hollow region and converge on the opposite side. The Detonation Shock Dynamics (DSD) model allows for the calculation of detonation propagation in a region of explosive using a selection of material input parameters, amongst which is the D-K relation that governs how the local detonation velocity varies as a function of wave curvature. In this paper, experimental data are compared to calculations using the newly-developed 3D DSD code at AWE with a variety of D-K relations. The effects of D-K variation through different calibration methods, material lot and initial density are investigated.

4:45PM R5.00005 Detonation performance of high-dense BTF charges. ALEXANDER DOLGOBORODOV, MICHAEL BRAZHNIKOV, MICHAEL MAKHOV, ICP RAS, SERGEY GUBIN, IRINA MAKLASSOVA, National Research Nuclear University “MEPhI” — New experimental data on detonation wave parameters and explosive performance for benzonitrifuroxan (BTX) are presented. Optical pyrometry was applied in order to measure the temperature and pressure of BTX detonation products. Chapman-Jouguet pressure and temperature were obtained as following: 33.8 GPa and 3990 K, 34.5 GPa and 4170 K (initial charge densities 1.82 and 1.84 g/cc respectively), the polytropic exponent was estimated as 2.8. The heat of explosion and acceleration ability were measured also. The results of calorimetric measurements performed in bomb calorimeter indicate that BTF slightly surpasses HMX in the heat of explosion. However BTF is inferior to HMX in the acceleration ability, measured by the method of copper casing expansion. It is also considered the hypothesis of formation of nanocarbon particles in detonation products directly behind the detonation front and influence of this processes on the temperature-time history in detonation products. The results of calculations with in view of formation of liquid nanocarbon in products of a detonation also are presented.
5:00PM R5.00006 Effects of confinement conditions on the detonation properties of vapor-deposited hexanitroazobenzene films, ROBERT KNEPPER, MICHAEL MARQUEZ, ALEXANDER TAPPAN, Sandia National Laboratories — It is well known that confining an explosive with a high-density inert material can cause substantial changes in its detonation properties. However, the thickness of confinement needed and the magnitude of the effect on quantities such as detonation velocity and critical thickness are largely unknown. In this work, we present vapor-deposited hexanitroazobenzene (HNAB) and copper films as a model system to study the effects of confinement on the detonation properties of secondary explosives. HNAB is chosen for the reproducibility of both its microstructure and detonation velocity when vapor-deposited, as well as its small critical thickness and the low surface roughness of the deposited films. Both the HNAB and copper confinement layers are vapor-deposited to promote intimate contact between the explosive and confinement and to provide precise control over both layer thicknesses and microstructure. Confinement thickness is varied to determine the minimum necessary to behave as though the confinement was effectively infinite, and the effects on detonation properties are quantified. These experiments may also provide insight into the structure of the detonation reaction zone by using the infinite confinement conditions (thickness and shock speed) to give an indirect measure of the reaction zone length.

5:15PM R5.00007 On the Partially Reacted Boundary Layer in Rate Sticks, YEHUDA PARTOM, Retired — Using our reactive flow model TDRR to simulate detonation in a rate stick, we observe that a partially reacted layer (PRL) is formed near the boundary. We are not aware that such a PRL has been observed in tests, and this is why we regarded it in the past as a numerical artifact. Assuming that such an artifact may be caused by the finite rise time of the detonation shock, we showed in [1] how it can be eliminated by delaying the outward boundary motion for a length — Using our reactive flow model TDRR to simulate detonation in a rate sticks, we observe that a partially reacted layer (PRL) is formed near the boundary. We may be caused by the finite rise time of the detonation shock, we showed in [1] how it can be eliminated by delaying the outward boundary motion for a length

Wednesday, July 10, 2013 3:30PM - 5:30PM — Session R6 TM Continuum Modeling I Cascade II - Amanual Teweldebrhan, Lawrence Livermore National Laboratory

3:30PM R6.00001 Equation of State for Shock Compression of High Distension Solids, DENNIS GRADY, Applied Research Associates — Shock Hugoniot data for full-density and porous compounds of boron carbide, silicon dioxide, tantalum pentoxide, uranium dioxide and play alluvium are investigated for the purpose of equation-of-state representation of intense shock compression. Complications of multivalued Hugoniot behavior characteristic of highly distended solids are addressed through the application of enthalpy-based equations of state of the form originally proposed by Rice and Walsh in the late 1950’s. Additivity of cold and thermal pressure intrinsic to the Mie-Gruneisen EOS framework is replaced by isobaric additive functions of the cold and thermal specific volume components in the enthalpy-based formulation. Additionally, experimental evidence supports acceleration of shock-induced phase transformation on the Hugoniot with increasing levels of initial distention for silicon dioxide, uranium dioxide and possibly boron carbide. Methods for addressing this experimentally observed facet of the shock compression are introduced into the EOS model.

4:00PM R6.00002 A Dynamic Discrete Dislocation Plasticity Method for the Dimulation of Plastic Relaxation under Shock Loading1, BENAT GURRUTXAGA-LERMA, Centre for Doctoral Training in Theory and Simulation of Materials, Imperial College London, ADRIAN P. SUTTON, DANIEL E. EAKINS, Department of Physics, Imperial College London, DANIEL S. BALINT, DANIELE DINI, Department of Mechanical Engineering, Imperial College London — This talk intends to offer some insight as to how Discrete Dislocation Plasticity (DDP) can be adapted to simulate plastic relaxation processes under weak shock loading and high strain rates. In those circumstances, dislocations are believed to be the main cause of plastic relaxation in crystalline solids. Direct simulation of dislocations as the dynamic agents of plastic relaxation in those cases remains a challenge. DDP, where dislocations are modelled as discrete discontinuities in elastic continuum media, is often unable to adequately simulate plastic relaxation because it treats dislocation motion quasi-statically, thus neglecting the time-dependent nature of the elastic fields and assuming that they

4:15PM R6.00003 Numerical simulation of multiscale damage-failure transition and shock wave propagation in metals and ceramics, YURIY BAYANDIN, NATALIA SAVELIEVA, Institute of continuous media mechanics of Ural branch of RAS, Russia, PERM — Statistical theory of evolution of typical mesoscopic defects revealed specific type of criticality-structural-scaling transitions and allowed the development of phenomenology of damage and plastic flow in materials under intensive loading, which established characteristic multiscale collective modes of defects responsible for formation of plastic waves and damage-failure transition. Original approach based on wide range constitutive equations was developed for simulation of multiscale damage-failure transition mechanisms and shock wave propagation in metals and ceramics in range of strain rate \(10^3 - 10^6 \text{s}^{-1}\). It was shown that mechanisms of a plastic relaxation and damage-failure transitions are linked to multiscale kinetics of meso-in defects collective modes with the nature of solitary waves and blow-up dissipative structures consequently. Numerical simulation of original plate impact tests showed that the model describes shock wave loading for metals and ceramics, and allowed us to explain the effect of power law phenomena of plastic waves fronts formation, its self-similar features under reloading and unloading. Analysis of shock wave profiles in ceramics for different thicknesses of specimens in terms of self-similar variables supports the universality of shock wave fronts.

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1 EPSRC CDT in Theory and Simulation of Materials

2 Research was supported by the Russian Foundation for Basic Research (projects N 11-01-00712, N 13-01-96034) and the program of fundamental research of Ural Branch of RAS (project N 12-P-1-1021).
4:30PM R6.00004 Jetting Instability Mechanisms of Particles from Explosive Dispersal. ROBERT RIPLEY, Martec Limited — The formation of post-detonation “particle” jets is widely observed in many problems associated with explosive dispersion of granular materials and liquids. Jets have been shown to form very early, however the mechanism controlling the number of jetting instabilities remains unresolved despite a number of active theories. Recent experiments involving cylindrical charges with a range of central explosive masses for dispersal of dry solid particles and pure liquid are used to formulate macroscopic numerical models for jet formation and growth. The number of jets is strongly related to the dominant perturbation during the shock interaction timescale that controls the initial fracturing of the particle bed and liquid bulk. Perturbations may originate at the interfaces between explosive, shock-dispersed media, and outer edge of the charge due to Richtmyer-Meshkov instabilities. The inner boundary controls the number of major structures, while the outer boundary may introduce additional overlapping structures and microjets that are overtaken by the major structures. In practice, each interface may feature a thin casing material that breaks up, thereby influencing or possibly dominating the instabilities. Hydrocode simulation is used to examine the role of each interface in conjunction with casing effects on the perturbation leading to jet initiation. The subsequent formation of coherent jet structures requires dense multiphase flow of particles and droplets that interact though inelastic collision, agglomeration, and turbulent interaction. Macroscopic multiphase flow simulation shows clustering of particles and merging of smaller instabilities with major jet structures. The methods are further applicable to particles premixed with explosive, which are known to form jets only with an external interface. Late-time dispersal is controlled by particle drag and evaporation of droplets. Numerical results for clustering and jetting evolution are compared with experiments. The work is extended to include interaction of particle and droplet jets with surrounding obstacles and associated combustion phenomena.

5:00PM R6.00005 Kinetic of phase transformation nucleated from grain boundaries . JEAN-BERNARD MAILLET, BERTRAND ROUET-LEDUC, CHRISTOPHE DENOUAL, CEA DAM, CEA DAM TEAM — A model for phase transitions initiated at nucleation sites on grain boundaries is proposed and tested against numerical simulations: a mean field approach allows to explicitly consider the granular structure, yielding accurate predictions for a wide span of nucleation processes. The transition between heterogeneous (i.e. controlled by the microstructure) and homogeneous behavior is predicted, which depends on the nucleation rate and the velocity of phase transformation.

5:15PM R6.00006 An Empirically Based Shaped Charge Jet Break-Up Model . ERNEST BAKER, JAMES PHAM, TAN VUONG, US Army ARDEC — This paper discusses an empirically based shaped charge jet break-up model based around Walsh’s break-up theory and provides significant experimental confirmation over a broad range of velocity gradients. The parameters which affect jet length and breakup times are fairly well known, but there is some controversy over the exact nature of the dependencies. Walsh theorized that the dependence of jet length would take a particular form, based on his determination of a dimensionless parameter for the problem and numerical experiments in which initial perturbation strengths were varied. Walsh did not present comparisons with experimental results. Chou has presented a variety of different jet break-up models with some data comparisons. Mostert [3] has suggested that breakup time is proportional to $\left(\frac{\Delta m}{\Delta v}\right)^{1/3}$. It is shown here that the parameter $\left(\frac{\Delta m}{\Delta v}\right)^{1/3}$ or $\left(\frac{\Delta m}{\Delta v}\right)^{1/3}$, closely related to Walsh’s dimensionless parameter, whose values were obtained from either experiments or simulations correlates quite well with jet breakup times for a very wide variety of shaped charge devices. The values of $\Delta m$ and $\Delta v$ are respectively the jet mass and the velocity difference of the portion of jet in question. For a typical shaped charge $\frac{\Delta m}{\Delta v}$ is essentially invariant with respect to time. In this paper, we present the mathematical basis for an empirically based break-up model with a similar basis to Walsh and Mostert, as well as supporting empirical data for a broad range of shaped charge geometries.

Wednesday, July 10, 2013 3:30PM - 5:15PM –
Session R7 CM.1 Equation of State: Modeling, Sponsored Invited Talk

3:30PM R7.00001 Recent developments in ab initio equations of state for ICF applications . LORIN BENEDICT, Lawrence Livermore National Laboratory — I present a brief review of recent work that we at Lawrence Livermore National Laboratory have conducted on the development of accurate EOS models for DT fuel, as well as for two candidate ablabor materials: Glow Discharge Polymer, and diamond. Emphasis will be placed on the use of ab initio electronic structure methods in producing data with which the EOS models are fit, as well as details of the EOS models themselves. Also discussed is the use of a variety of experimental data in the validation of these models.

3:45PM R7.00002 Useful microscopic concepts for high pressure phenomena1. J. MANUEL RECIO, J. MANUEL MENÉNDEZ, RUTH ÁLVAREZ-URÍA, MIRIAM MARQUÉS, Malta-Consolider Team and Universidad de Oviedo, TARIK QAHARANI, University Abubakr Belkaid, VALENTIN G. BAONZA, Malta-Consolider Team and Universidad Complutense de Madrid — A better understanding of the macroscopic behavior of crystalline solids under pressure can be achieved introducing microscopic concepts as the local compressibility ($\kappa_i = -\frac{\partial V}{\partial p}$) and the local pressure ($p_i = -\frac{\partial E}{\partial V}$). Both are derived from topological analysis of crystalline electron densities. This formalism allows for a partition of the unit cell volume ($V$) into disjoint atomic-like regions such that $V = \sum V_i$, $i$ runs over all different atomic constituents. Using this topological partition, the compressibility of the crystal is recovered: $\kappa = \sum \frac{1}{V_i} \kappa_i$. Although local pressures are not additive, their reciprocals are: $\frac{1}{p} = \sum \frac{1}{V_i}$, where $p$ is the thermodynamic pressure. This fact leads to the interpretation of the atomic constituents of crystals as parallel mechanical resistors when pressure is applied. Consequently, atomic-like mechanical resistances and mechanical conductances can be defined. After extensive first principles calculations, computed results of these local properties reveal systematic trends for crystal families under pressure, as we illustrate for II-VI binary semiconductors and oxide spinels.

1 Funded by Spanish MINECO and MICINN through CSD2007-00045 and CTQ2012-38599 projects.

4:00PM R7.00003 Multiphase Equations of State for Structural Materials at High Pressures1. KONSTANTIN V. KHISCHENKO, IJHT RAS, Moscow, Russia — Equations of state for materials over a wide range of pressures and temperatures are needed for numerical simulations of processes in shock-compressed media. Accuracy of calculation results is determined mainly by adequacy of equation of state of a medium. In this work, a new multiphase equation-of-state model is proposed with taking into account the polymorphic phase transformations, melting, evaporation and ionization. Thermodynamic calculations are carried out for metals, alkali halides, and polymer materials in a broad region of the phase diagram. Obtained results are presented in comparison with available data of experiments at high dynamic pressures in shock and release waves.

1 This work is supported by RFBR, grant 11-08-01225
4:15PM R7.00004 Shock Invariants and Conservation Laws in (1+1) Dimensions, ROGER MINCH, DANIEL ORLIKOWSKI, GEORGE LEVESQUE, LLNL — The origin of scaling laws in shocked condensed matter is blessed by a number of new techniques and facilities that are shattering previous experimental limitations: static pressures above 600 GPa, equation of state (EOS) experiments on pulsed-power machines, picosecond-resolved x-ray diffraction on free-electron lasers, and many new experiments on high-energy lasers. Our goals, using high-energy lasers, have been to push the limits of high pressure accessible to measurement and to bridge the gap between static- and dynamic-compression experiments by exploring off-Hugoniot states. I will review laser techniques for both shock- and ramp-compression experiments, and discuss a variety of diagnostics. I will present recent results including: impedance-matching Hugoniot experiments, absolute-Hugoniot implosive-shock radiography, coupled radiometry and velocimetry, ramp-compression EOS, and in-situ x-ray diffraction and absorption spectroscopy into the TPa regime. As the National Ignition Facility (NIF) transitions to a laser user facility for basic and applied science, we are transferring many of these techniques. The unprecedented quality and variety of diagnostics available, coupled with exquisite pulse-shaping predictability and control make the NIF a premier facility for extreme-compression experiments.

4:30PM R7.00005 Role of anharmonicity in the phonon contribution to the Grüneisen parameter, R. RAVELO, University of Texas, El Paso, TX, B.L. HOLIAN, Los Alamos National Laboratory, Los Alamos, NM — The Grüneisen parameter $\gamma$ is directly related to the thermal expansion of a solid and to its equation of state (EOS). Several formulations of $\gamma$ based on the isothermal EOS and pressure derivatives of elastic moduli have been developed over the years and predict different values for $\gamma$ at zero pressure and its pressure dependence. The uncertainty in these “mechanical” models can be addressed by density functional theory (DFT) calculations using the Mie-Grüneisen formulation in which the vibrational contribution to the pressure is treated within the quasi-harmonic approximation while the static contribution is accounted by the cold curve. However, the vibrational Grüneisen need not agree with either the thermodynamic value or any of the mechanical models, and is in fact overestimated in transition metals. We examine the difference between the vibrational and thermodynamic Grüneisen parameter employing both classical molecular dynamics and lattice dynamics and utilizing classical interatomic potentials for bcc and fcc crystals constructed to have similar elastic moduli and cold curves but with different degrees of anharmonicity and transverse and longitudinal Brillouin edge zone phonon frequencies.

4:45PM R7.00006 Characterization of Earth Mantle Materials, GABRIEL GWNMESIA, Delaware State University

Thursday, July 11, 2013 8:00AM - 9:00AM –
Session S1 Plenary Session IV Grand Ballroom I - Choong-Shik Yoo, Washington State University

8:00AM S1.00001 Laser Driven, Extreme Compression Science, JON EGGERT, Lawrence Livermore National Laboratory — Extreme-compression science is blessed by a number of new techniques and facilities that are shattering previous experimental limitations: static pressures above 600 GPa, equation of state (EOS) experiments on pulsed-power machines, picosecond-resolved x-ray diffraction on free-electron lasers, and many new experiments on high-energy lasers. Our goals, using high-energy lasers, have been to push the limits of high pressure accessible to measurement and to bridge the gap between static- and dynamic-compression experiments by exploring off-Hugoniot states. I will review laser techniques for both shock- and ramp-compression experiments, and discuss a variety of diagnostics. I will present recent results including: impedance-matching Hugoniot experiments, absolute-Hugoniot implosive-shock radiography, coupled radiometry and velocimetry, ramp-compression EOS, and in-situ x-ray diffraction and absorption spectroscopy into the TPa regime. As the National Ignition Facility (NIF) transitions to a laser user facility for basic and applied science, we are transferring many of these techniques. The unprecedented quality and variety of diagnostics available, coupled with exquisite pulse-shaping predictability and control make the NIF a premier facility for extreme-compression experiments.

Thursday, July 11, 2013 9:15AM - 10:45AM —
Session T1 ME.3 Inelastic Deformation, Fracture, and Spall VIII Grand Ballroom III - Sunil Dwivedi, Georgia Institute of Technology

9:15AM T1.00001 ABSTRACT WITHDRAWN —

9:30AM T1.00002 Modeling the Plastic Response of Single Crystals to High Strain Rate Deformation, CURT BRONKHORST, Los Alamos National Laboratory, BENJAMIN HANSEN, University of New Mexico, IRENE BEYERLEIN, ELLEN CERRETA, DARCIE DENNIS-KOLLER, Los Alamos National Laboratory — A new metallic single crystal model based upon statistical average dislocation interactions is presented. This model includes motion of dislocations becoming drag-limited rather than thermally activated, requiring a physical transition in the average dislocation motion with strain-rate. Based upon the dislocation dynamics work of Wang, Beyerlein, and Lesar, plastic deformation evolution is based on statistical dislocation populations and the evolution of those populations. Three main dislocation populations are considered: 1) glissile dislocations ($\rho_D$); 2) glissile dislocations, which currently do not move referred to as “pile up” ($\rho_P$), and 3) sessile dislocations ($\rho_S$). Mobile dislocations ($\rho_D$) move through the crystal and are blocked by obstacles, react and annihilate, react and become sessile, or exit the region. The motivation to model the distribution of dislocation velocities is used to create the simplest distribution of two populations moving at two velocities. Results of single-crystal tensile simulations using the new model at various rates are compared to copper experiments. The key findings are: 1) a single-crystal model capable of transitioning from low to high strain rates, and 2) prediction of the transition from thermally activated to drag-dominated strain rates. Further investigation is easily adaptable in the model.

9:45AM T1.00003 The release of shear stress in metals under dynamic loading, RADE VIGNJEVIC, Cranfield University, NEIL BOURNE, AWE, Aldermaston — Metals under shock loading relieve shear stress by slip after. This work focuses on the types of loading where a metal initially responds entirely elastically and plasticity with deformation mechanisms developing over time and determined by the material’s state and microstructure. Finite kinetics in shock is mirrored in several commonly observed responses including elastic precursor decay and the measurement of shear stress histories during load. FCC and BCC metals have different kinetics, with those of BCC metals slower. A model, under development, is implemented here to depict the behaviour observed by assigning a finite time to the return of the state point from the quasi equilibrium yield surface to the equilibrium yield surface. This delays the softening of the material and reproduces observed response in the weak shock regime. The model is based on the assumption that formation and self-organisation of dislocation structures at various scales maximises dissipation rate (minimize the free energy) in the material. Initial validation of the model is performed on tantalum by comparing stress histories under shock and shock-less loading with experimental data in order to assess its ability to reproduce experimentally observed features.
10:00AM T1.00004 Response of FCC and BCC Metals to High-Amplitude Dynamic Compression, MARC MEYERS, UC San Diego, BRUCE REMINGTON, BRIAN MADDOX, Lawrence Livermore National Laboratory, EDUARDO BRINGA, Universidad Nacional de Cuyo, Argentina, HYE-SOOK PARK, Lawrence Livermore National Laboratory, CHIA-HUI LU, UC San Diego — The experimentally observed response of FCC and BCC metals to high-amplitude compressive waves is compared with analytical predictions using constitutive models based on dislocations and twinning and with molecular dynamics simulations. In FCC metals (Cu and Ni), the predictions of dislocation densities from a homogeneous nucleation model are close to those of molecular dynamics simulations. Both are orders of magnitude higher than experimentally observed residual dislocation densities. MD calculations predict a drastic decrease in dislocation densities upon unloading, bringing the values in agreement with measurements. For BCC metals (Ta), on the residual densities are close to predictions of Orowan dislocation multiplication. Due to the much higher Peierls-Nabarro stress, the MD simulations predict much lower dislocation densities than in FCC metals subjected to similar pressures. At higher amplitudes, both FCC and BCC metals experience extensive twinning. The threshold pressure for twinning is successfully modeled by constitutive model based on a critical shear stress for twinning, at the imposed strain rate and temperature. Research funded by UCOP/UC Labs Program.

10:15AM T1.00005 Phase transformations coupled to deformation processes, TURAB LOOKMAN, Los Alamos National Laboratory — Phase transformation processes have a substantial impact on the inelastic and damage response of materials. Yet, our understanding of how different loading conditions affect volume fractions of transformed phases, microstructure and transformation pathways is very much in its infancy. With an emphasis on distilling single crystal physics that can, in principle, be incorporated into higher length scale models, I will discuss how recent atomistic simulations on Ti are beginning to provide insights into transformation pathways and the interplay of phase transformations and deformation processes. These simulations are complemented by shock experiments on Zr, Ti together with characterization studies at the Advanced Photon Source.

Thursday, July 11, 2013 9:15AM - 10:30AM Session T2 CM.4 Warm Dense Matter II Elliott Bay - Hae-Ja Lee, LCLS, SLAC National Acceleration Laboratory

9:15AM T2.00001 Development of quasi-isentropic drives to 500 GPa and beyond, SHON T. PRISBREY, HYE-SOOK PARK, BRIAN MADDOX, BRUCE REMINGTON, ROBERT CAVALLO, MARK MAY, TOM ARSENLIS, Lawrence Livermore National Laboratory — The ability to reliably measure materials at energy densities exceeding 5x10^11 J/m^3 (500 GPa) requires an experimental platform that reaches such energy densities in a controlled manner and in a configuration that allows measurements to occur. We have developed a staged shock drive that will quasi-isentropically ramp materials such as Ta and Mo into such a high energy density state and simultaneously keep the materials substantially below their melting point, i.e., in their solid phase. Recent measurements of our platform on the National Ignition Facility have confirmed our ability to predict the resultant drive with a peak pressure of ~500 GPa. Separate experiments at the same facility have recently demonstrated that a drive with peak pressures >800 GPa is possible. We will show the experimental platform, the simulated and measured drives produced by the platform for ~500 GPa and ~800 GPa drive shots. We will also show an experimental platform which utilizes the drive and measurements of the samples to infer material strength. This work was performed under the auspices of the Lawrence Livermore National Security, LLC, (LLNS) under Contract No. DE-AC52-07NA27344. LLNL-ABS-620612

9:30AM T2.00002 Absolute equation of state and opacity measurements of CH plastic to 40 TPa using the National Ignition Facility1, T. DOEPNER, D.C. SWIFT, J.A. HAWRELIAK, A. KRITCHER, G.W. COLLINS, S. GLENZER, Lawrence Livermore National Laboratory, S.D. ROTHMAN, D. CHAPMAN, AWE Aldermaston, J. GAFFNEY, S. ROSE, Imperial College, London, R. FALCONE, University of California - Berkeley — We have developed an experimental configuration using a hohlraum-driven spherically-convergent shock to induce pressures into the gigabar range, measuring the Hugoniot radiographically. The shock pressure increases with convergence, so a range of Hugoniot states is obtained from a single experiment. The opacity along the Hugoniot is also deduced, which is essential in gigabar experiments as it changes significantly from its initial value. We are focusing initially on plastics, as we can reliably obtain spherical samples with the desired design of ablator, and the radiographic signal is reasonable. Our initial measurements on NIF used a conservative timing of the x-ray backlighter to allow for uncertainty in the EOS, and probed only part of the pressure range. The shock speed and compression, obtained from radiographic analysis, gave absolute Hugoniot states from 12-41 TPa, which is an order of magnitude greater than previously measured in CH. The measured EOS locus was consistent with the previous measurements, and significantly stiffer than the theoretical EOS used for comparison. Our analysis also gave the variation of opacity along the Hugoniot, which showed a decrease of an order of magnitude, as expected from atomic physics calculations.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

9:45AM T2.00003 Non equilibrium studies on FEL facilities, MARION HARMAND, LULI, ecole polytechnique, 91128 Palaiseau, France — The recent development of Free Electron Lasers (FEL), giving ultrafast, high intensity pulses in the X-ray and XUV energy range is opening new opportunities for WDM studies. Development of X-ray diagnostics such as X-ray absorption spectroscopy and X-ray scattering, has received much attention for the in situ measurement of the structural and physical properties of matter at extreme conditions [1]. Coupled to ultrafast pump - probe schemas, such diagnostics are giving new insights into out-of-equilibrium processes and thus validate current models. We report recent developments to perform few fs time resolved pump - probe experiments [2], giving access to ultrafast transient WDM states. We also present collective Thomson Scattering with soft x-ray Free Electron Laser radiation (at FLASH) as a method to track the evolution of highly transient warm dense hydrogen with around 100 fs time resolution. In addition, recent experiments at LCLS are suggesting the possibility to perform X-ray absorption spectroscopy (XANES) on FEL facilities to provide simultaneous information on the valence electrons and on the atomic local arrangement within sub-ps time scales.


10:15AM T2.00004 Ultrafast XFEL diffraction measurements of femtosecond laser-driven shock-compressed iron, TOMOKAZU SANO, NORIMASA OZAKI, TOMOKI MATSUDA, RYOTA KASHIWABARA, NORIHITO MATSUYAMA, HIROYUKI URAISHI, KAZUKI NAKATSUKA, YOSHIHITO KONDO, TAKEKI MATSUOKA, Osaka University, YUJI SANO, Toshiba Corporation, YOSHIHIKO TANGE, Ehime University, TOMOKO SATO, TOSHIHITO SEKINE, Hiroshima University, KAZUTO ARAKAWA, Shimane University, TADASHI TANAKA, KENSUKE TONO, MAKINA YABASHI, RIKEN, OSAMI SAKATA, National Institute for Materials Science, AKIO HIROSE, RYOHIKO KODAMA, Osaka University — We measured lattice dynamics under femtosecond laser-driven shock-compressed phase transition in iron using X-ray free electron laser with sub-picosecond temporal resolution. Sluggish behavior of iron under shock-induced bcc to hcp transition is the unsolved issue although the diffusionless type of structural transition should be completed within picoseconds. We performed in-situ XRD at SPring-8 Angstrom Compact free electron Laser (SACLA) facility to take a series of snapshots of diffraction patterns under the transition in iron using XFEL pulse with pulse duration of 10 fs varying the delay time from the pumping femtosecond laser pulse. The evolution of lattice defects and high-pressure phase will be addressed in the talk.

10:15AM T2.00005 Response of FCC and BCC Metals to High-Amplitude Dynamic Compression, MARC MEYERS, UC San Diego, BRUCE REMINGTON, BRIAN MADDOX, Lawrence Livermore National Laboratory, EDUARDO BRINGA, Universidad Nacional de Cuyo, Argentina, HYE-SOOK PARK, Lawrence Livermore National Laboratory, CHIA-HUI LU, UC San Diego — The experimentally observed response of FCC and BCC metals to high-amplitude compressive waves is compared with analytical predictions using constitutive models based on dislocations and twinning and with molecular dynamics simulations. In FCC metals (Cu and Ni), the predictions of dislocation densities from a homogeneous nucleation model are close to those of molecular dynamics simulations. Both are orders of magnitude higher than experimentally observed residual dislocation densities. MD calculations predict a drastic decrease in dislocation densities upon unloading, bringing the values in agreement with measurements. For BCC metals (Ta), on the residual densities are close to predictions of Orowan dislocation multiplication. Due to the much higher Peierls-Nabarro stress, the MD simulations predict much lower dislocation densities than in FCC metals subjected to similar pressures. At higher amplitudes, both FCC and BCC metals experience extensive twinning. The threshold pressure for twinning is successfully modeled by constitutive model based on a critical shear stress for twinning, at the imposed strain rate and temperature. Research funded by UCOP/UC Labs Program.
9:15AM T3.00001 High-pressure and temperature investigations of energetic materials. JARED GUMP, Naval Surface Warfare Center, Indian Head Division — Static high-pressure measurements are extremely useful for obtaining thermodynamic and phase stability information from a wide variety of materials. However, studying energetic materials can be challenging when extracting information from static high-pressure measurements. Energetic materials are traditionally C, H, N, O compounds with low crystalline symmetry, producing weak signal in commonly performed x-ray diffraction measurements. The small sample volume available in a static high-pressure cell exacerbates this issue. Additionally, typical hydrostatic compression media, such as methanol/ethanol, may react with many energetic materials. However, characterization of their thermodynamic parameters and phase stability is critical to understanding explosive performance and sensitivity. Crystalline properties, such as bulk modulus and thermal expansion, are necessary to accurately predict the behavior of shocked solids using hydrodynamic codes. In order to obtain these values, equations of state of various energetic materials were investigated using synchrotron angle-dispersive x-ray diffraction experiments at static high-pressure and temperature. Intense synchrotron radiation overcomes the weak x-ray scattering of energetic materials in a pressure cell. The samples were hydrostatically compressed using a non-reactive hydrostatic medium and heated using a heated diamond anvil cell. Pressure-volume data for the materials were fit to the Birch-Murugan and Vinet formalisms to obtain bulk modulus and its first pressure derivative. Temperature-volume data at ambient pressure were fit to obtain the thermal expansion coefficient. Data from several energetic materials will be presented and compared.

9:45AM T3.00002 The high pressure-temperature phase behavior of 2,4,6-trinitrotoluene (TNT). PATRICK BOWDEN, RAJA CHELLAPPA, DANA DATTELBAUM, VIRGINIA MANNER, NATHAN MACK, Los Alamos National Laboratory, ZHENXIAN LIU, Brookhaven National Laboratory — 2,4,6-trinitrotoluene (TNT) is a widely used explosive that is relatively insensitive to initiation by shock loading. While the detonation properties of TNT have been extensively reported, the high pressure–temperature (P–T) stability of TNT has not been investigated in detail. In addition, there are no studies that have determined the effects of pressure on the stability of the liquid phase. At ambient conditions, TNT crystallizes in a monoclinic lattice (space group Pca2_1). In this work, we have performed in situ synchrotron XRD and vibrational spectroscopy measurements at various P–T conditions along isothermal and isobaric pathways to confirm previously reported phase transitions, and investigate phase stabilities up to 30 GPa and 500 °C. Using all the available data, we have established the first comprehensive high P–T phase diagram of TNT, including the melting line as a function of pressure. While our synchrotron IR and Raman spectroscopy measurements indicate spectral changes at ∼2 GPa, careful XRD measurements (hydrostatic, He medium and non-hydrostatic) reveal that the monoclinic phase is likely stable up to 20 GPa. We will present a self-consistent P–V–T equation of state derived from the reported structural and vibrational data.

10:00AM T3.00003 High Pressure-Temperature Phase Diagram of 1,1-diamino-2,2-dinitroethylene. MATTHEW BISHOP, RAJA CHELLAPPA, Los Alamos National Laboratory, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington, DANIEL PRESTON, MARY SANDSTROM, DANA DATTELBAUM, Los Alamos National Laboratory, YOGESH VOHRA, University of Alabama at Birmingham, NENAD VELISAVLJEVIC, Los Alamos National Laboratory — 1,1-diamino-2,2-dinitroethylene (FOX-7) is a less sensitive energetic material with performance comparable to commonly used secondary explosives such as RDX and HMX. At ambient pressure, FOX-7 exhibits complex polymorphism with at least three structurally distinct phases (α, β, and γ). In this study, we have investigated the high P–T stability of FOX-7 polymorphs using synchrotron mid-infrared (MIR) spectroscopy. At ambient pressure, our MIR spectra confirmed the known α → β (110 °C) and β → γ (160 °C) phase transitions; as well as, indicated an additional phase transition, γ → δ (210 °C), with the δ phase being stable up to 250 °C prior to melt/decomposition. In situ MIR spectra obtained during isobaric heating at 0.9 GPa revealed that the α → β transition occurs at 180 °C, while β → δ phase transition shifted to 300°C with suppression of γ phase. Decomposition was observed above 325°C. Based on multiple high P–T measurements, we have established the first high P–T phase diagram of FOX-7.

2This work was, in part, supported by the US DOE under contract No. DE-AC52-06NA25396 and Science Campaign 2 Program. MB acknowledges additional support from the NSF BD program. Use of NSLS (DE-AC02-08CH11144) and beamline U2A (COMPRES, No.EAR01-35554, CDAC).

10:15AM T3.00004 High pressure stability of hydrazine (H₂N-NH₂): Implications for energetic hydronitrogen compounds. RAJA CHELLAPPA, DANA DATTELBAUM, Los Alamos National Laboratory, ZHENXIAN LIU, U2A Beamline, National Synchrotron Light Source — Hydrazine (H₂N-NH₂) is a metastable, high energy density molecule that is relevant to planetary physics and plays an important role in industrial synthesis and propellant applications. Theoretical calculations have predicted the existence of “hydronitrogen” extended solids that hold great potential as a high energy density material (HEDM). Exploring the high pressure-temperature (P–T) stability of hydrazine will provide crucial insights into hydrogen bonded -N-H networks under these conditions. Further, related simple molecules such as CH₄, NH₃, CO, and CO₂ have been shown to have rich high P–T phase diagrams, often forming extended amorphous solids. Here, we report the first comprehensive study of hydrazine to 50 GPa at ambient temperature, using both in situ vibrational spectroscopy and synchrotron x-ray diffraction to elucidate structural changes driven by compression. Liquid hydrazide solidifies into a monoclinic structure at 0.5 GPa that is isomorphous with the low-T solid phase. Further compression drives structural re-ordering and at least 2 phase transformations to 20 GPa, with complex anisotropic hydrogen bonding interactions. Surprisingly, no evidence for the formation of extended amorphous solids was observed to the highest pressure studied.

10:30AM T3.00005 Double Shock Experiments and Reactive Flow Modeling on LX-17 to Understand the Reacted Equation of State. KEVIN S. VANDERSALL, FRANK GARCIA, LAURENCE E. FRIED, CRAIG M. TARVER, Lawrence Livermore National Laboratory — Experimental data from measurements of the reacted state of an energetic material are desired to incorporate reacted states in modeling by computer codes. In a case such as LX-17 (92.5% TATB and 7.5% Kel-F by weight), where the time dependent kinetics of reaction is still not fully understood and the reacted state may evolve over time, this information becomes even more vital. Experiments were performed to measure the reacted state of LX-17 using a double shock method involving the use of two flyer materials (with known properties) mounted on the projectile that send an initial shock through the material close to or above the Chapman-Jouguet (CJ) state followed by a second shock at a higher magnitude into the detonated material. By measuring the parameters of the first and second shock waves, information on the reacted state can be obtained. The LX-17 detonation reaction zone profiles plus the arrival times and amplitudes of reflected shocks in LX-17 detonation reaction products were measured using Photonic Doppler Velocimetry (PDV) probes and an aluminum foil coated LiF window. A discussion of this work will include the experimental parameters, velocimetry profiles, data interpretation, reactive CHEETAH and Ignition and Growth modeling, as well as possible future experiments. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
Thursday, July 11, 2013 9:15AM - 10:45AM –
Session T4 **NT.2** Novel Techniques: Velocity diagnostics  
Vashon - Scott Jackson, Los Alamos National Laboratory

9:15AM T4.00001 Measurement of an Explosively Driven Hemispherical Shell Using 96 Points of Optical Velocimetry  
JEREMY DANIELSON, EDWARD DAYKIN, Los Alamos National Laboratory, ABEL DIAZ, National Security Technologies, DEAN DOTY, Los Alamos National Laboratory, BRENT FROGGET, National Security Technologies, MIKE FURLANETTO, Los Alamos National Laboratory, CENOBIO CALLEGOS, MIKE GIBO, ANSELMO GARZA, National Security Technologies, DAVID HOLTKAMP, Los Alamos National Laboratory, MANDY HUTCHINS, National Security Technologies, CANDACE JOGERST, Los Alamos National Laboratory, CARLOS PEREZ, MIKE PENA, VINCENT ROMERO, National Security Technologies, MIKE SHINAS, Los Alamos National Laboratory, MATT TEEL, National Security Technologies, LENNY TABAKA, Los Alamos National Laboratory — We report the measurement of the surface motion of a hemispherical copper shell driven by high explosives. This measurement was made using four 32 channel multiplexed photonic Doppler velocimetry (PDV) systems, in combination with a novel compound optical probe. Clearly visible are detailed features of the motion of the shell over time, enhanced by spatial correlation. Significant non-normal motion is apparent, and challenges in measuring such a geometry are discussed.

9:30AM T4.00002 A multi-point radial photonic Doppler velocimetry (PDV) diagnostic for cylindrical implosion experiments  
DEVON DALTON, DANIEL DOLAN, RAYMOND LEMKE, RYAN MCBRIDE, MATTHEW MARTIN, ERIC HARDING, Sandia National Laboratories, SCOTT WALKER, National Security Technologies — Radial photonic Doppler velocimetry (PDV) has been successfully applied in cylindrical implosion experiments fielded on Sandia’s Z accelerator. Magnetically driven cylinders have been diagnosed well beyond 20 km/s, using a “leapfrog” configuration to address the bandwidth limitations of currently available detectors and digitizers. Implosion symmetry is the latest question this diagnostic will attempt to answer. An innovative multi-point configuration is being developed to allow six concurrent measurements during each experiment. This presentation describes the implementation of radial PDV in this extreme environment. Sandia National Labs is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Dept. of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:45AM T4.00003 Optical distance measurements to recover the material approach missed by optical velocimetry  
MATTHEW BRIGGS, Los Alamos National Laboratory, DAN KNERRIM, Tektronix, ERIK MORO, SHAWN MCGRANE, Los Alamos National Laboratory — Optical velocimetry is limited to measuring the component of the target velocity along the axis of the optical beam, thereby allowing a laterally moving tilted surface to approach a probe undetected. In some applications it is important to know the distance to the target surface, and the forgoing means that integrating the velocity can give incorrect calculations of position. We will present three approaches to overcome this limitation: Tilted wavefront interferometry to map time of flight into fringe displacement; pulse bursts for which we measure the change in the average arrival time of a burst, and amplitude modulation interferometry in which a change in path length shows up as a change in the phase of the modulation. All three of these have the potential to be integrated with existing velocimetry probes for simultaneous velocity and displacement measurements. We will also report on initial tests of these approaches. LAUR - 13-21022

10:00AM T4.00004 Optical pins for sub-nanosecond resolution of detonation break out  
MIKHAIL SHINAS, MATTHEW BRIGGS, MICHAEL ARCHULETA, Los Alamos National Laboratory — We report on the design and tests of optical pins that we have shown to resolve the arrival of a detonation front with a resolution of <1ns. We coat the end of single-mode fiber with a 1000 Ångström layer of aluminum and butt it against a detonator in various locations. Using an IR interferometer with the reference leg shifted in frequency (the type used for Photon Doppler Velocimetry), the disappearance of the fringes allows a measurement of the arrival of the detonation front to ~200 ps. The detonation arrival time measured with the optical pin and IR interferometer agree within the resolution of the measurement. A more fieldable and affordable alternative using APDs Avalanche photodiodes to measure the disappearance of the light reflected from the aluminum coating yields a resolution of 1ns. We present the design details and performance proof tests. LA-UR - 13-21216

10:15AM T4.00005 In-situ polymer strain diagnostics using mecanochemical sensor molecules  
JOSEPH HOOPER, PATRICK SMITH, Naval Postgraduate School, JAMES HEMMER, JAVIER READ DE ALANIZ, University of California, Santa Barbara, BRIAN MASON, JOEL CARNEY, Naval Surface Warfare Center, Indian Head Division — We report the synthesis and initial high-strain rate response of polymer materials with embedded force-sensitive molecules. PMA, PMMA, and HTPB were polymerized directly off a spiropyran molecule which undergoes a reversible ring-opening transition upon the application of local stress from the polymer chains. Following the transition there is a distinct change in color, UV response, and vibrational spectra as the spiropyran opens into a merocyanine form similar to many fluorescent dyes. In principle, these sensor molecules allow mapping of local strains with extremely high resolution and no perturbation of overall mechanical properties. However, this transition process has previously only been studied at very low quasi-stationary strain-rates, and was shown to be strongly affected by the nature of the polymer matrix, proximity to the glass transition, and other factors. We present the first dynamic loading experiments on these mecanochromic polymers using gas-gun and Hopkinson bar compression. Initial results on soft, elastomeric polymer matrices suggest widespread activation of the sensor molecule at high strain-rates, but that alternate synthesis and materials preparation strategies may be required to decouple the strain activation from straight thermal activation.

1Support provided by DTRA Basic Research

10:30AM T4.00006 Preliminary Investigations of HE Performance Characterization Using SWIFT  
MICHAEL MURPHY, CARL JOHNSON, Los Alamos National Laboratory — Initial pseudo-aquarium experimentation is underway to assess the utility of using the shock wave image framing technique (SWIFT) to characterize HE performance on detonator length and time scales. SWIFT is employed to directly visualize shock waves driven into polymethylmethacrylate (PMMA) samples through detonation interaction in pseudo-aquarium test geometries. Columns of XTX 8004, an extrudable RDX-based high explosive, are either cured directly within PMMA dynamic witness plates or within confinement tubes of different materials with varying shock impedances that are then embedded within PMMA. For current experiments, the SWIFT system records 16-frame image sequences using 175 ns inter-frame delays to directly visualize the evolution of lead shock front geometries as they are driven radially into PMMA by the detonating XTX column. Standard aquarium-test analysis is employed to calculate shock pressure evolution within PMMA, and detonation wave velocities are accurately calculated from the time-resolved images as well. The SWIFT system and numerous pseudo-aquarium experimental results will be presented and discussed.

Thursday, July 11, 2013 9:15AM - 10:30AM –
Session T5 **T5.2** Continuum Modeling II  
Cascade I - Turab Lookman, Los Alamos National Laboratory
9:15AM T5.00001 A design of experiments approach for sensitivity screening of mesoscale simulations of explosive impact. GEORGE BUTLER, AFRL/RWME/TEAS, JOHN COX, AFRL/RWME, TERESA DAILY, AFRL/RWWL, KEITH GONTHIER, LSU — This paper discusses a Design of Experiments (DOE) approach for planning inert mesoscale simulations to establish how microstructure and composition affect the uniaxial impact sensitivity of metalized Plastic Bonded Explosives (PBXs). Simulations are performed using an explicit, 2D, cohesive finite and discrete element code (CODEX), developed at Georgia Institute of Technology, and account for nonlinear deformation and fracture of PBXs: explosive crystals (HMX) and aluminum particles (Al) in a polymeric binder. The relative sensitivity of PBX formulations is established by critical hot-spots formed in the microstructure. The code has flexibility in prescribing material properties, but this initial screening examines five independent variables: impact speed, initial size of HMX crystals and Al particles, and initial volume fractions of HMX and Al (the binder ensures saturation). Input settings are prescribed by the DOE approach, which plans the experiments to ensure an ability to reach statistically valid, objective conclusions with minimal runs. A full factorial matrix of simulations requires 296 runs, and each run takes up to a week. DOE reduced the matrix to 101 runs, while retaining the ability to estimate dominant variable effects and the effect of variable interactions on hot spot formation. These analyses provide a qualitative validation of CODEX, and a framework for subsequent simulations. DISTRIBUTION A. Approved for public release, distribution unlimited. (96ABW-2013-0054)

9:30AM T5.00002 Modeling and analysis of high-explosive driven perturbed plate experiments at Los Alamos. JAMES COOLEY, RUSSEL OLSON, DAVID ORO, Los Alamos National Laboratory — Measurement and modeling of fluid instabilities has been an important part of numerical simulation verification and validation efforts from the beginning of computational fluid dynamics. The use of these same instabilities to assess the accuracy and validity of models for material strength began at least by the middle of the 1970s [1]. These techniques have been improved upon over many decades, for example recent work in Russia [2]. These techniques have proven useful in challenging various different models for material response. We have performed several experiments at the Los Alamos pRad facility for perturbation growth in both Tantalum and Depleted Uranium. These results provide excellent data images over several microseconds of growth. In this paper, we will present efforts to use these experiments to validate our numerical code and constitutive models. We will detail a systematic study of various constitutive models for the metals and evaluate the rigidity of the constraint that these experiments provide to the modeling community. We will spend some time examining the assumptions in the constitutive models and assessing the relative uncertainties of each major assumption. LA-UR 13-21726.


9:45AM T5.00003 Modeling of propellant flow and explosively-driven valve for the Large-Bore Powder Gun. KIN LAM, Los Alamos National Laboratory — The Large-Bore Powder Gun, with a 3.5-inch bore, is being developed to provide dynamic experiments on physics samples at the Nevada Test Site with impact velocities exceeding 2 km/s. A confinement system is required to seal the target chamber from the gun system to keep it free of hazardous materials from the impact event. A key component of the confinement system is an explosively driven valve (EDV), which uses a small amount of explosive (PBX 9501) to drive an aluminum piston perpendicular to the barrel axis into a tapered hole. The objective of this study is to evaluate the efficiency of the EDV design via computational simulations using models validated with prototype experiments. We first established the gun performance characteristics using an interior ballistics code. Then an energy source model capable of generating the kinematics (i.e., pressure, velocity and displacement profiles) as predicted by the interior ballistic code is used in the hydrodynamics code CTH to calculate the M14 propellant gas expansion as the projectile travels down the gun barrel with the goal of obtaining the lateral (stagnation) pressure load on the EDV piston as it is inserted into the bore. A model of the EDV operation validated against stand-alone experiments is also developed. The gas flow and EDV models are combined to simulate integrated tests as well as the operating conditions specified for qualification. Results from these simulations and those involving design modifications to improve the confinement will be presented.

10:00AM T5.00004 Multiple necking during dynamic extension of round bar: linear stability approach versus finite element calculations. SKANDER EL MAI, CEA, France, JACQUES PETIT, CEA, France, ALAIN MOLINARI, Universite de Lorraine, France — The fragmentation of structures has been widely investigated in the literature, with experimental, numerical or analytical works. Many authors have proposed to reproduce by FEA the experimental fragmentation process by introducing for instance a perturbation to trigger instabilities. Therefore, the authors were able to capture the distribution of fragments. Few of them are interested in the characterization of the onset time of instability. In the proposed contribution, the multiple necking of a round bar in dynamic tensile loading is analysed by the finite element method. A perturbation of the initial flow stress is introduced in the numerical model. Various levels of loading velocities and of perturbation amplitudes are considered. The onset time of localized instabilities ti and the number of necks Nn have been characterized. A logarithmic dependence of variables ti and Nn with the loading velocity is shown. The time ti is observed to depend strongly on the level of the perturbations introduced in the numerical model while the number of necks Nn evolves moderately. Besides, by defining salient criteria in terms of the growth rate of the perturbation, a comparison of linear stability analysis dedicated to multiple necking with the numerical results can be performed. A good correlation in terms of onset time of instabilities and of number of necks is shown.

10:15AM T5.00005 Dynamic Response of Viscoelastic Plates to High Pressure Induced by Bubble Collapse. S.W. GONG, E. KLASEBOER, J. LOU, Institute of High Performance Computing, Singapore — The numerical simulations of viscoelastic plates to high pressure induced by underwater explosion bubble will be presented in this paper. The boundary-element method (BEM) is used to simulate the physical process of the explosive bubble growth, contraction and collapse. The finite element method (FEM) is used to calculate the viscoelastic plates response to the high pressure induced by underwater explosion bubble. The interaction of the viscoelastic plates and the underwater explosion bubble is simulated numerically via the coupled BEM-FEM. The computational procedure for the prediction of dynamic response of the viscoelastic plates to the high pressure induced by underwater explosion bubble is demonstrated. The case studies are conducted to examine the effects of different charge weights and locations on dynamic response of the viscoelastic plate. The results from this study may provide some insights into to the problem of viscoelastic structures subjected to underwater explosion bubble, which might be useful for potential applications in biomedicine or marine industry.

Thursday, July 11, 2013 9:15AM - 10:30AM – Session T6 ME.3 Inelastic Deformation, Fracture, and Spall XIII Cascade II - Zbig Dreger, Washington State University
9:15AM T6.00001 Influence of Grain Boundary Properties on Spall Strength, SARYU FENSIN, STEVE VALONE, ELLEN CERRETA, GEORGE GRAY, Los Alamos National Laboratory — There are many factors thought to affect the spall strength of a grain boundary, including: grain boundary structure, energy, and excess volume, in addition to its interactions with dislocations. In this work, we explore the affect of average and local properties on the spall strength of a grain boundary. The average properties explored in this work include grain boundary energy and excess volume while local properties include plastic work at grain boundary. Flyer plate simulations were carried out for five boundary types with different structures, energies and excess volume. These boundaries were chosen as model systems to represent various boundaries observed in “real” materials. Simulations indicate that there is no direct correlation between the spall strength of a boundary and either its energy and excess volume. This result suggests that average properties of grain boundaries alone are not sufficient indicators of the spall strength of a boundary and perhaps local boundary properties need to be taken into account to predict boundary spall strength. In fact, better correlation was found between the ability of a boundary to undergo plastic deformation and spall strength.

9:30AM T6.00002 On the dynamic tensile strength of zirconium, GARETH APPLEBY-THOMAS, AMER HAMED, RADE VIGNJEVIC, Cranfield University, CLIVE SIVIOUR, University of Oxford, PAUL HAZELL, University of New South Wales, JONATHAN PAINTER, Cranfield University — Dynamic tensile failure (spall) initiation via cracks, voids, etc, before subsequent coalesces, is known to be highly microstructure-dependent. In particular, the availability of slip planes and other methods of plastic deformation controls the onset (or lack thereof) of spall. While studies have been undertaken into the spall response of BCC and FCC materials, less attention has been paid to spall of highly anisotropic HCP materials. Here the dynamic behaviour of zirconium is investigated via plate-impact experiments, with the aim of building on an on-going in-house body of work investigating this complex class of materials. In particular, in this paper the effects of impact stress, pulse duration and texture on spall have been interrogated using velocimetry techniques.

9:45AM T6.00003 Ballistic properties of debris produced by laser shock-induced micro-spallation of tin samples, DIDIER LOISON, THIBAUT DE RESSEGUIER, ANDRE DRAGON, Institut P’ - CNRS UPR 3346 - ISAE-ENSMA, DPMMatt Team — Dynamic fragmentation in the liquid state after melting under shock compression or upon release leads to the ejection of a cloud of droplets. This phenomenon, called micro-spallation, remains essentially unexplored in most metals. We present laser shock experiments performed on tin, to pressures ranging from about 60 to 220 GPa. Experimental diagnostics include skew Photonic Doppler Velocimetry (PDV) measurements of the droplets velocities, transverse observations of the expanding cloud of droplets, and soft recovery of ejecta within a low density gel. Optical microscopy of the gel reveals the presence of droplets which confirm shock-induced melting prior to fragmentation. To quantify size distribution of the debris, 3D X-ray micro-tomography has been performed at the ESRF synchrotron facility in France (similar to US Advanced Photon Source), where sub-micrometer resolution could be achieved. In this paper, the resulting velocity and size distributions are presented and compared with theoretical predictions based on a one-dimensional description accounting for laser shock loading, wave propagation, phase transformations, and fragmentation. Discrepancies between measured and calculated distributions are discussed. Finally, combining size and velocity data provides estimates of the ballistic properties of debris and their kinetic energy, which are key issues for anticipating the damage produced by their impacts on nearby equipments.

10:00AM T6.00004 Study on metal ejection under laser shock loading, XIN JIANTING, GU YUQIU, Chinese Academy of Engineering Physics — Dynamic response of metal to shock loading plays an important role in the fields of civil engineering, aeronautics etc. The loading method of intense laser driven shock wave has many advantages to study the ejection process. The present work is devoted to laser shock experiments in metal ejection, and get access to fragments recovery and post-test evaluation of the fragment-size distribution. The experiments were carried out on the SGII laser facility, the samples are tin foil of 106µm and 260 µm. Two high power pulsed laser beams of 0.532 µm wavelength are focused onto the target, the laser beams were homogenized by cpp, and the irradiated spot is quasi circular with 2nm diameter. The dynamic fragmentation were recovered by CH foam with 200mg/cm3 density. One dimensional simulations were performed with HYADES code, and the pressures near the free surface of the targets driven by laser in experiments are 13Gpa, 27Gpa, 42Gpa and 50Gpa respectively. We observed the fragments in the CH foam tube by X-ray radiographs and CT image reconstruction. The total number and characteristic size of fragments have been detected.

10:15AM T6.00005 Experimental and Numerical Study of Water-Filled Vessel Impacted by Flat Projectiles, WEI ZHANG, PENG REN, WEI HUANG, YUBO GAO, Harbin Institute of Technology — To understand the failure patterns and impact resistance of watertight vessel, a flat-nosed projectile was accelerated by a two–stage light gas gun against a vessel filled with water which was placed in experiments are 13Gpa, 27Gpa, 42Gpa and 50Gpa respectively. We observed the fragments in the CH foam tube by X-ray radiographs and CT image reconstruction. The total number and characteristic size of fragments have been detected.

9:15AM T7.00001 Low-temperature high-pressure spectroscopy in Co2+-doped ZnO: effects of crystal structure and dimensionality, CARLOS RENERO-LECUINA, RAFAEL VALIENTE, MALTA-CONSOLIDER Team - Dpt. Applied Physics, Univ. of Cantabria, Spain, JESUS GONZALEZ, FERNANDO RODRIGUEZ, MALTA-CONSOLIDER Team - DCITIMAC, Univ. of Cantabria, Spain, ROSA MARTIN-RODRIGUEZ, Cond. Mater. & Interfaces, Debye Institute for NanoMaterials Science, Utrecht Univ. The Netherlands, GLORIA ALMONACID-CABALLER, ALFREDO SEGURA, MALTA-CONSOLIDER Team - ICMUV, Univ. of Valencia, Spain, VICENTE MARIN-BORRAS, VICENTE MUÑOZ-SANJOSÉ, ICMUV, Univ. of Valencia, Spain — Wide band-gap semiconductors doped with transition-metal ions have attracted a lot of attention in the past few years. Here we focus on the spectroscopic properties of Co2+-doped ZnO in different structural conformations such as single crystal, thin film, nanorods and nanoparticles under different P − T conditions. Optical measurements were obtained by means of Raman and time-resolved spectroscopy using high-pressure techniques. Our main goal is to investigate the pressure-induced Wurtzite-to-Rock-Salt phase transition and how the structural conformation affects the Raman spectra as well as the absorption and emission spectra associated with Co2+-doped ZnO. The effects of quantum confinement (dimensionality) are also investigated through the distinct spectral features observed in the samples as SC, TF, NW and NP helping us to clarify the still-unassigned absorption and emission spectra in terms of electron-phonon couplings and exchange interactions.

**Thursday, July 11, 2013 9:15AM - 10:30AM — Session T7 CM.2 Phase Transitions: Structural Transitions II**

Grand Crescent - Stan Tozer, National High Magnetic Field Laboratory
and the first principles total energy calculations. XeF
K.CoF
magnetoresistance, exotic magnetism, or even high T
a wide multidisciplinary science. Perovskite or distorted-perovskite oxides are relevant as solid state devices as many of them exhibit properties such as colossal magnetoresistance, exotic magnetism, or even high Tc superconductivity. In geoscience, the understanding of high-pressure postperovskite phase is noteworthy. In this sense, it must be noted that NaCoF3 transforms to the postperovskite phase at a moderate pressure (P ≈ 15 GPa) in comparison to oxides [1]. However KCoF3 seems to lack this transition as it remains in the perovskite structure up to higher pressure [2]. This work reports a structural study in KCoF3 as a function of pressure in the 0-60 GPa range. Its large pressure perovskite stability is noteworthy. Therefore, this is a unique system to establish correlations between crystal and electronic structures in a high-symmetry phase, where Co2+ ions are located in a perfect octahedral environment. Here we present an x-ray diffraction study in correlation with single-crystal optical absorption spectroscopy. The variation of the crystal-field strength and Racah parameters of Co2+
with the crystal volume (and Co-F distance) up to 60 GPa are presented, discussed and compared with available data in other structures involving oxides and chlorides.

9:45AM T7.00003 X-ray diffraction study of amorphous lithium disilicate glass processed under high pressure, ALTAIR SORIA PEREIRA, SILVIO BUCHNER, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil, JOAO CARDOSO DE LIMA, Universidade Federal de Santa Catarina, Florianopolis, SC, Brazil, NAIRA MARIA BALZARETTI, Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil — Lithium disilicate glass (Li2O:2SiO2) is a very interesting vitreous material, because, besides several important technological applications (e.g. biomaterial to produce prostheses and implants), shows a large difference between the Tg and Tc values. This is important for the investigation of the crystallization mechanism on vitreous phases, as it allows the independent study of the nucleation and growth stages. In this work, we have investigated the effect of high-pressure processing in the induction of structural changes in the amorphous phase. This can give place to polymorphism and/or to the generation of possible seeds for a crystalline phase nucleation. Using toroidal type high-pressure chambers, glass samples were processed at 2.5 GPa, 4 GPa, 6 GPa and 7.7 GPa at room temperature. Synchrotron X-ray diffraction was used to obtain the radial distribution functions (RDF), in order to follow the structural changes at different ranges. Compared to a pristine sample, the main change observed for the samples processed up to 6 GPa was associated to the distortion of the SiO4 tetrahedra, as already observed in the literature. However, for the sample processed at 7.7 GPa, we have identified a drastic change in the RDF which points for the production of a different amorphous phase with a local structure closer to that observed for the Li2SiO4 crystalline phase.

10:00AM T7.00004 Cs in high oxidation states and as a p-block element, MAOSHENG MIAO, University of California Santa Barbara — A long time doctrine rooted in the atomic shell model states that the atoms maintain a complete inner shell while interacting with other atoms. Therefore, group IA elements, for example, are invariably stable in the +1 charge state because the p electrons of their inner shells do not react with other chemical species. This general rule governs our understanding of the structures and reactions of matter and has never been challenged. In this work, I will show for the first time a striking result that while mixing with fluorine under pressure, Cs atoms will share their 5p electrons and become oxidized to a higher charge state. It forms stable CsF3 compounds, consisting of neutral or ionic CsF3 molecules. Their geometry and bonding resemble isoelectronic XeF6 molecules, showing that Cs chemically behaves like a p-block element. The stability of these remarkable compounds will change the understanding of the periodic table and chemistry of elements. The work was done by using an automatic crystal structure search based on particle swarm optimization algorithm and the first principles total energy calculations.

10:15AM T7.00005 The consequences of the pressure-induced spinel – post spinel transition upon the electronic properties of MgFe2O4, MARK NIKOLAEVSKY, ERAN GRINBERG, WEIMING XU, GREGORY KH. ROSENBERG, MOSHE P. PASTERNAK, School of Physics and Astronomy, Tel Aviv University, AVIVA MALCHIOR, Nuclear Research Center Negev. Similar to maghemite, the ferrimagnetic manganese-iron (SG Fd3m, T_N ≈ 710 K) is a four-spin ferromagnetic manganese-iron (SG Fd3m, T_N ≈ 710 K) is a four-spin structure. The A and B sites are 4- and 6-fold coordinated moieties, respectively. At ~25 GPa a 14 order structural transition takes place into a denser, the so called, post-spinel (ps) structure. The few studies carried out so far concluded that the ps structure is either of the CaMn2O4 or CaTi2O4-type. Our preliminary HP Mössbauer studies (MS) have unambiguously revealed two Fe sites contradicting the one Fe-site typical of the CaMn2O4 or the CaTi2O4 polymorphs. This presentation describes the evolution of the electronic/magnetic properties of the ps phase of MgFe2O4 up to 80 GPa. Experiments at variable-T were carried out with MS and electrical resistance at both at compression and decompression. At 47 GPa (> P_t > P_s) the Mössbauer spectra reveals a paramagnetic state at RT composed of two -quadrupole-split sites, which are crystallographically ordered at T > T_C (≈ 320 K). Two fully magnetic split components are present at T < P_s (~ 53 K), R (P, 300 K) R(P) increases sharply reaching a peak at 20 GPa and drops continuously by 10^-6 at P > 50 GPa. By decomposition to ~ 4 GPa the electronic/magnetic properties remain typical of the ps phase.

Supported by the ISF grant # 789/10

Thursday, July 11, 2013 11:00AM - 12:30PM
Session U1 ME.3 Inelastic Deformation, Fracture, and Spall IX Grand Ballroom III - Oleg Naimark, Russian Academy of Sciences

11:00AM U1.00001 Interpreting the shock response of porous oxide systems, DAVID FREDBURG, DARCIE KOLLER, Los Alamos National Laboratory — Oxide powders subjected to varying levels of shock loading can exhibit a complex response that differs significantly from that which is commonly observed in metals. As much of the early model development for particulates has been focused on metallic systems, the current state of the art in compaction and equation of state modeling is often unable to capture the wide range of compression responses observed in porous oxides. Specifically, the possibility of polymorphic phase transformations requires additional considerations in the development of compaction and equation of state models for these systems. In the present work, the shock response of several porous oxide systems is critically examined with respect to the equilibrium and metastable state models for these systems. Post shock XRD measurement of transformation.

11:15AM U1.00002 Dynamic yield and tensile strengths of spark plasma sintered alumina, INNA GIRLITSKY, E. ZARETSKY, S. KALABUKHOV, M. DARIEL, N. FRAGE, Ben-Gurion University — Fully dense alumina samples with 0.6-µm grain size were produced from alumina powder using Spark Plasma Sintering and tested in two types of VISAR-instrumented planar impact tests. . In the tests of the first type the samples of 0.28 to 6-mm thickness were loaded by 1-mm tungsten impactors accelerated up to velocity of about 1 km/s. These tests were aimed to study of the Hugoniot elastic limit (HEL) of the SPS-processed alumina and the decay of the elastic precursor wave with the propagation distance. In the second type of the tests the samples of ~ 3-mm thickness were loaded by 1-mm copper impactors accelerated up to velocities 100-1000 m/s was. These tests were aimed to study the dynamic tensile (spall) strength of the alumina. The data on the decay of the elastic precursor wave allow determining the rates of the irreversible (inelastic) strains in the SPS-processed alumina at the initial stages of the shock-induced plastic deformation and, thus, to derive some conclusions concerning the mechanisms responsible of the deformation. The data on the tensile fracture of the alumina demonstrate a monotonous decline of the spall strength with the amplitude of the loading stress pulse.
**11:30 AM U1.00003 Impact Simulations for a Pre-Stressed Ceramic**, JAMES CAZAMIAS, DRC, STEPHAN BILYK, ARL, MICHAEL KORNECKI, DSI — Applying a pre-stress to a ceramic using confinement increases the initial strength and ductility and helps suppress tensile failure. This confinement is not necessarily hydrostatic, so deviatoric pre-stresses may also be introduced. Although experimental testing of confined ceramic is becoming more common, numerical modeling of ceramic response in these configurations has been limited. We have developed a methodology to examine shrink-fit configurations using ALE3D. Experiments are conducted to examine the effects of ceramic confinement when impacted with projectile rods, and we are modeling these experiments using this methodology and the Johnson-Holmquist-Beissel model.

**11:45 AM U1.00004 Low Pressure Shock Hugoniot of Silica Aerogel**, RICKY CHAU, LLNL — We present measurements on the low pressure shock Hugoniot of silica aerogel. Previous measurements of the shock Hugoniot of silica aerogel give a Hugoniot that when extrapolated to 10 GPa pressures give unphysical results. In this study, we used photonic Doppler velocimetry to measure the shock transit time in silica aerogel. The new shock Hugoniot data show a turnover in the shock Hugoniot of silica aerogel at low pressures. The turnover resolves the unphysical behavior in the shock Hugoniot. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

**12:00 PM U1.00005 Deformation Behaviour of Coarse Grain Alumina under Shock Loading**, SATISH GUPTA, Applied Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085 — To develop better understanding of the shock wave induced deformation behavior of coarse grain alumina ceramics, and for measurement of its Hugoniot Elastic Limit (HEL), in-situ and recovery gas gun experiments have been carried out on coarse grain alumina (grain size ~ 10 µm), prepared in the form of discs (>99.9% TMD) by pressure-less sintering of alpha alumina powder at 1583 K. The HEL value of 1.9 GPa has been determined from the kink in the pressure history recorded using piezoresistance gauge and also from the free surface velocity history of the sample shocked to 9 GPa. The nano-indentation measurements on the alumina samples shocked to 6.5 GPa showed hardness value 15% lower than 21.3 GPa for unshocked alumina, and strong Indentation Size Effect (ISE); the hardness value was still lower and the ISE was stronger for the sample shocked to 12 GPa. The XRD measurements showed reduced particle size and increased microstrains in the shocked alumina fragments. SEM, FESEM and TEM measurements on shock treated samples showed presence of grain localized micro- and nano-scale deformations, micro-cleavages, grain-boundary microcracks, extensive shear induced deformations, and localized micro-fractures, etc. These observations led to the development of a qualitative model for the damage initiation and its subsequent growth mechanisms in shocked alumina. The work performed in collaboration with K.D. Joshi of BARC and A.K. Mukhopadhyay of CGCRI.

**Thursday, July 11, 2013 11:00AM - 12:30PM — Session U2 NT.1 Novel Techniques: Spectroscopy**

**11:00 AM U2.00001 Coherent Raman Studies of Shocked Liquids**, SHAWN MCGRANE, KATHRYN BROWN, NHAN DANG, CYNTHIA BOLME, DAVID MOORE, Los Alamos National Laboratory — Transient vibrational spectrometers offer the potential to directly observe time dependent shock induced chemical reaction kinetics. We report recent experiments that couple a hybrid picosecond/femtosecond coherent anti-Stokes Raman spectroscopy (CARS) diagnostic with our tabletop ultrafast laser driven shock platform. Initial results on liquids shocked to 20 GPa suggest that sub-picosecond dephasing at high pressure and temperature may limit the application of this nonresonant background free version of CARS. Initial results using interferometric CARS to increase sensitivity and overcome these limitations will be presented.

**11:15 AM U2.00002 Picosecond Dynamics of Shock Compressed and Flash-Heated Nanometer Thick Films of HMX**1, CHRISTOPHER BERG, DANA DLOTT, University of Illinois at Urbana-Champaign — New results are described for probing molecular dynamics of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) subjected to shock compression to a few GPa and/or temperature excursions exceeding thermal decomposition values (T > 500K). 5-10 nm thick films of δ-HMX were grown on metallic substrates coated with monolayers of 4-nitrothiophenol. Due to shock velocities of a few nm/ps, nanometer thick films allowed picosecond time resolution of shock loading. A plastic polymer layer a few microns in thickness was spin-coated on top of HMX for shock confinement purposes. Both the monolayer and explosive layer were probed utilizing an ultrafast nonlinear coherent vibrational spectroscopy, vibrational sum-frequency generation. Shock compression pressures were estimated via comparison of the monolayer nitro transition frequency shift with static high pressure measurements in a diamond anvil cell. Temperature determinations were based on thermoreflectance measurements of the metallic substrate.

1 Supported by the Stewardship Sciences Academic Alliance Program from the Carnegie-DOE Alliance Center under grant number DOE CIW 4-3253-13 and the US Air Force Office of Scientific Research under award number FA9550-09-1-0163.

**11:30 AM U2.00003 In Situ Investigation of the Dynamic Response of Energetic Materials using IMPULSE at the Advanced Photon Source**, KYLE RAMOS, Los Alamos National Laboratory — The mechanical and chemical response of energetic materials is controlled by spatial heterogeneity and crystalline mechanics that evolve during impact. Traditional methods use continuum measurements to infer the microstructure response whereas advances in synchrotron capabilities and diagnostics are providing new, unique opportunities to interrogate materials in real time and in situ. Recently the IMPULSE team has performed experiments on a gas-gun system (IMPact system for Ultrafast Synchrotron Experiments) using single X-ray bunch phase contrast imaging (PCI) and Laue diffraction at the Advanced Photon Source (APS) to examine shock-induced phenomena in energetic materials and other inert, molecular analogues. The low absorption of molecular materials maximizes x-ray beam penetration, allowing measurements in transmission using the brilliance currently available at APS Sector 32. The transmission geometry enables exciting possibilities for observing both average lattice response and spatially heterogeneous, continuum response (2 um spatial resolution, 60 ps exposure, 153ns frame-rate) in energetic materials ranging from single crystals to plastic bonded composites. This capability provides a means for linking mechanics with detonation initiation by resolving deformation mechanisms such as compaction, void collapse and jetting, cracking, dislocation-mediated plasticity and phase transformation. Representative data will be presented and discussed to illustrate current progress and future directions for this new technology.
12:00PM U2.00004 Laser-driven flyer plates for shock compression spectroscopy

1. DANA DLOTT, WILLIAM SHAW, ALEXANDER CURTIS, ALEXANDR BANISHEV, University of Illinois at Urbana-Champaign — A laser-driven mini flyer plate system was developed for shock compression spectroscopy. A commercial one-box 2J YAG laser produces a homogeneous top hat beam with a diffraction optic. An 8 GHz PDV characterizes flyer velocity profiles up to 5 km/s. Flyers are routinely launched with velocities reproducible to +1-1%, and the 1 mm diameter flyers have enough energy to initiate energetic materials. High-speed spectroscopic diagnostics have been synchronized. Design elements such as diameter, thickness, laser pulse duration, substrate size, and so on will be discussed. Illustrations will be presented, including monitoring shock front structures with embedded optical gauges and understanding mechanisms of reactive nanomaterial impact initiation.

2 Supported by ARO W911NF-10-1-0072, AFOSR FA9550-09-1-0163, DTRA HDTRA1-12-1-0011 and NNSA Carnegie-DOE Alliance Center DOE CIW 3-3253-13.


12:15PM U2.00005 High resolution Broadband CARS of laser shocked materials

1. BRUCE BAER, BRIAN MADDOX, Lawrence Livermore National Laboratory — We will present preliminary data and methods detailing experiments scheduled later this year using Janus at the Jupiter Laser Facility at LLNL to obtain Coherent Anti-stokes Raman Spectra (CARS) of materials under shock conditions. High resolution (~1 cm−1) CARS of the pre-shocked materials will demonstrate the feasibility and high precision of the methods involved. Pressures as high as 200 GPa have been previously achieved. Initially, our experiments will focus on quartz and diamond and should subsequently lead to hydrogen, deuterium and other constituents of the giant gas planets.

This work has been supported under the auspices of the U.S. Department of Energy under Contract DE-AC52-07NA27344.

Thursday, July 11, 2013 11:00AM - 12:30PM –
Session U3 EM.1 Energetic Materials Equation of State II
Fifth Avenue - Seth Root, Sandia National Laboratories

11:00AM U3.00001 Plate impact experiments on the TATB based explosive PBX 9502 at pressures near the Chapman-Jouguet state

1. R.L. GUSTAVSEN, T.D. ASLAM, B.D. BARTRAM, B.C. HOLLOWELL, Los Alamos National Laboratory — We have completed a series of two-stage gas-gun driven plate-impact experiments on PBX 9502 (95 wt.% tri-amino-trinitro-benzene, 5 wt.% Kel-F800 plastic binder). The ultimate goal of these experiments is to provide, in the neighborhood of the Chapman-Jouguet state, overdriven product data for use in the JWL equation of state. The authors present results of determination of sound velocities in explosion products of PBX 9502.

11:15AM U3.00002 Equation of state of detonation products based on statistical mechanical theory

1. YANHONG ZHAO, HAIFENG LIU, GONGMU ZHANG, HAIFENG SONG, IAPCM (Institute of Applied Physics and Computational Mathematics), IAPCM TEAM — The equation of state (EOS) of gaseous detonation products is calculated using Ross’s modification of hard-sphere variation theory and the improved one-fluid van der Waals mixture model. The condensed phase of carbon is a mixture of graphite, diamond, graphite-like liquid and diamond-like liquid. For a mixed system of detonation products, the free energy minimization principle is used to calculate the equilibrium compositions of detonation products by solving chemical equilibrium equations. Meanwhile, a chemical equilibrium code is developed based on the theory proposed in this article, and then it is used in the three typical calculations as follow: (i) Calculation for detonation parameters of explosive, the calculated values of detonation velocity, the detonation pressure and the detonation temperature are in good agreement with experimental ones. (ii) Calculation for isentropic unloading line of RDX explosive, whose starting points is the CJ point. Comparison with the results of JWL EOS it is found that the calculated value of gamma is monotonically decreasing using the presented theory in this paper, while double peaks phenomenon appears using JWLEOS.

11:30AM U3.00003 Computations of fluid mixtures including solid carbon at chemical equilibrium

1. EMERIC BOURASSEAU, CEA — One of the key points of the understanding of detonation phenomena is the determination of equation of state of the detonation products mixture. Concerning carbon rich explosives, detonation products mixtures are composed of solid carbon nano-clusters immersed in a high density fluid phase. The study of such systems where both chemical and phase equilibriums occur simultaneously represents an important challenge and molecular simulation methods appear to be one of the more promising way to obtain some answers. In this talk, the Reaction Ensemble Monte Carlo (RxMC) method will be presented. This method allows the system to reach the chemical equilibrium of a mixture driven by a set of linearly independent chemical equations. Applied to detonation product mixtures, it allows the calculation of the chemical composition of the mixture and its thermodynamic properties. Moreover, an original model has been proposed to take explicitly into account a solid carbon meso-particle in thermodynamic and chemical equilibrium with the fluid. Finally our simulations show that the intrinsic inhomogeneous nature of the system (i.e. the fact that the solid phase is immersed in the fluid phase) has an important impact on the thermodynamic properties, and as a consequence must be taken into account.

12:00PM U3.00004 Determination of sound velocities of “overcompressed” detonation in HMX-based explosive

1. ALEXEY KOVALEV, MIKHAIL ZHERNOKLETOV, VLADIMIR BEL’SKY, EVGENY BOGDANOV, Russian Federal Nuclear Center - VNIIEF, VNIIEF TEAM — The authors present results of determination of sound velocities in explosion products (EP) of HMX-based explosive overcompressed up to the pressures of 50-85 GPa by overtaking unloading method. The radiowave and optical methods are used to record the time when front of overcompressed detonation wave in investigated sample of high explosive (HE) is overtaken by expansion wave, which propagates from the back surface of impactor with sound velocity. The data on sound velocities, which were independently obtained by two different methods, were in agreement. The methods with use of radiowave interferometer and indicator liquid are rather effective for determination of sound velocities in overcompressed EP and for investigation of parameters in the Jouget point of various HEs, which are required for calibration of their equations of state (EOS).
12:15PM U3.00005 Improved Relationships for the Thermodynamic Properties of Carbon Phases at Detonation Conditions, LEONARD STIEL, Polytechnic Institute of NYU (Retired), ERNEST BAKER, DANIEL MURPHY, U.S. Army ARDEC Picatinny Arsenal — In order to improve the procedures utilized in the Jaguar thermochemical program for carbon, volumetric and heat capacity relationships have been developed for graphite, diamond, and liquid carbon forms. Available experimental thermodynamic property and Hugoniot data have been analyzed to establish optimum equations of state for the carbon phases. The appropriate carbon form or multiple forms at equilibrium results from the minimization of the Gibbs free energy of the system. The resulting relationships are utilized to examine the phase behavior of carbon at elevated temperatures and pressures. The behavior of metastable carbon states is optimized by analyses of Hugoniot data for hydrocarbons, and C-J and cylinder velocities for a database of CHNO explosives. The accuracy of the resulting relationships is demonstrated by comparisons for several properties, including the Hugoniot behavior of oxygen-deficient explosives at overdriven conditions.

Thursday, July 11, 2013 11:00AM - 12:00PM –
Session U4 NM.3 Novel Properties III Vashon - J.M Recio, University of Oviedo

11:00AM U4.00001 Pressure Induced Superconductivity in Topological Compounds, CHANGQING JIN, Chinese Academy of Sciences — Topological quantum compounds attract worldwide attention because of many novel physical properties. Topological superconductivity is one of most excited topological quantum states since its surface supports Majorana fermions [1] that are assumed many new physics. We found superconductivity can be realized in a typical topological insulator Bi$_2$Te$_3$ induced via pressure above 3 GPa where the surface remains gapless Dirac cone[8]. The Hall coefficient measurements indicated carriers evolved as function of pressure. The x ray diffraction experiments at high pressure indicated that Bi$_2$Te$_3$ keeps stable up to 8GPa. This strongly suggests that the superconductivity observed in Bi$_2$Te$_3$ ambient phase is topological related. Acknowledgments: This work was supported by nsf & MOST of China.

References

11:30AM U4.00002 High Pressure High Temperature Devitrification of Iron-Based Metallic Glass, ANDREW STEMSHORN, YOGESH VOHRA, University of Alabama at Birmingham — High pressure high temperature devitrification of Fe$_72$B$_{15}$Si$_{9}$ metallic glass was studied by in situ energy dispersive x-ray powder diffraction measurements at HPCAT beamline 16BM-B, APS utilizing a portable Paris Edinburg cell with an integrated graphite heater. Structural changes were measured using sequential 20 second EDDX spectrums with white beam synchrotron x-ray incident radiation source. The iron-based metal glass sample along with MgO pressure standard was first pressurized and then heated at a constant rate of 2.5 K/min. Onset crystallization temperature is taken as the point where crystal peaks become apparent in the x-ray spectrum at twice the intensity of spectral noise. Heating is continued until the amorphous profile of the glass give way completely to crystalline peaks. This procedure was repeated for 0.2, 1.0, 2.0, 3.0, 4.5 and 6.0 GPa. The sample showed a marked increase in the onset of crystallization temperature with pressure, with 783 K at 0.2 GPa to 873 K at 6.0 GPa. The first phase to precipitate in each case is a bcc iron phase and other iron-boron and iron-silicon phases appeared at higher temperatures. The possibility of nucleating nanocrystalline phase was also investigated with the aim of forming a nano-composite material with enhanced mechanical properties.

11:45AM U4.00003 A novel assembly used for hot-shock consolidation, PENGWAN CHEN, QIANG ZHOU, Beijing Institute of Technology, STATE KEY LABORATORY OF EXPLOSION SCIENCE AND TECHNIQUE TEAM — A novel assembly characterized by an automatic set-up was developed for hot-shock consolidations of powders. The under-water shock wave and the high-temperature preheating, which are considered as two effective ways to eliminate cracks, were combined in the system. In this work, pure tungsten powders and tungsten-copper mixture were separately compacted using this new assembly. The pure tungsten powder with a grain size of 2µm were compacted to high density (96%T.D.) at 1300°C, and the 90W-10Cu (wt pct) mixtures were compacted to nearly theoretical density at 1000°C. The results showed that both samples were free of cracks. The consolidated specimens were then characterized by SEM analysis and micro-hardness testing.

Thursday, July 11, 2013 11:00AM - 12:30PM –
Session U5 TM Continuum Modeling III Cascade I - Robert Ripley, Martec Limited

11:00AM U5.00001 Analysis of Compaction Wave Dissipation in Porous Metalized Explosive$^1$, PRATAP RAO, KEITH GONTHIER, Mechanical and Industrial Engineering Department, Louisiana State University — It is well established that the inclusion of reactive metals in explosive formulations can enhance post-detonation energy release but it remains unclear, even for idealized systems, how the composition and microstructure of metal containing porous solid explosives affects dissipative heating within compaction waves that is important for weak initiation of detonation. In this study, we perform meso-scale simulations to computationally examine how the initial porosity and metal mass fraction of aluminized and microstructure of metal containing porous solid explosives affects dissipative heating within compaction waves that is important for weak initiation of detonation. In this study, we perform inert meso-scale simulations to computationally examine how the initial porosity and metal mass fraction of aluminized and

$^1$This research is supported by the Defense Threat Reduction Agency (DTRA) under sponsor award number HDTRA1-10-1-0018, and the Air Force Research Laboratory (AFRL-RWME) under sponsor award number FA8651-09-0021.
11:00AM U6.00001 Multiscale strength (MS) models: their foundation, their successes, and their challenges1, ROBERT RUDD, Lawrence Livermore National Lab — Multiscale strength (MS) models are constructed to capture a natural hierarchy in the deformation of metals such as V and Ta starting with atomic bonding and extending up through the mobility of individual dislocations, the evolution of dislocation networks and so on until the ultimate material response at the scale of an experiment. In practice, the hierarchy is described by quantum mechanics, molecular dynamics, dislocation dynamics, and so on, ultimately informing a continuum constitutive model. We review the basic models and describe their extension to plastic flow in shocked metals and the response of polycrystalline materials. In experimental systems that match the assumptions of the MS models, they work surprisingly well, both for fundamental experiments like in-situ single crystal diffraction, and for more integral experiments such as shock initiation and detonation phenomena, their extension to plastic flow in shocked metals and the response of polycrystalline materials. In experimental systems that match the assumptions of the MS models, they work surprisingly well, both for fundamental experiments like in-situ single crystal diffraction, and for more integral experiments like Rayleigh-Taylor plastic flow experiments. There are also clear challenges, however. The current MS models do not include failure, and they are expensive to create, due to the large amounts of computer time needed. Still, MS models provide compelling insight into metals under extreme pressures and strain rates.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
11:30 AM U6.00002 Strain anisotropy and shear strength of shock compressed tantalum measured from in-situ Laue diffraction

CHRISTOPHER WEHRENBERG, MATT TERRY, BRIAN MADDOX, Lawrence Livermore National Laboratory, ANDREW COMLEY, Atomic Weapons Establishment, HYE-SOOK PARK, SHON PRISBREY, JAMES HAWRELIJK, Lawrence Livermore National Laboratory, JUSTIN WARK, ANDREW HIGINBOTHAM, University of Oxford, BRUCE REMINGTON, Lawrence Livermore National Laboratory — Laser driven shock experiments, performed at the Omega facility, studied the dynamic yield strength and lattice dynamics of single crystal tantalum using in-situ Laue diffraction. Tantalum samples were shocked along the [100] direction to peak stresses up to 60 GPa and probed using the bremsstrahlung radiation from an imploding CH capsule x-ray source. Diffraction spots for both the undriven and driven regions of the sample were recorded simultaneously on time-integrated image plate detectors. The strain anisotropy was measured from the position shift of the driven diffraction spot and the total strain state was found using the volumetric strain from VISAR. Yield strength measurements were inferred from the data and compared with predictions from various models, including the LLNL multi-scale strength model for Ta.

1 This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

11:45 AM U6.00003 Investigations into rapid uniaxial compression of polycrystalline targets using femtosecond X-ray diffraction

DAVID McGONEGLE, ANDREW HIGINBOTHAM, SAM VINKO, JUSTIN WARK, University of Oxford, UK — When a material is uniaxially shock or ramp compressed to high pressures on ultrafast timescales, the rate at which the lattice response occurs can compete with the kinetics of the plasticity, and thus the material can deviate greatly from a hydrostatic response, and the assumption that the difference between the longitudinal and transverse strains in a sample remains small becomes increasingly invalid. We present analysis of X-ray diffraction data from laser shocked polycrystalline targets subjected to large strains, as well as large strain anisotropies, factors of which many existing models fail to correctly take account. We demonstrate that by breaking the symmetry of the experiment, using a tilted target geometry, it is possible to measure these strain anisotropies in a polycrystal. We present data acquired using this technique performed on the MEC beamline at LCLS, and discuss possible future experiments, such as investigations into the Voigt-Reuss parameter using such emerging 4th generation light sources.

12:00 PM U6.00004 ABSTRACT WITHDRAWN —

Thursday, July 11, 2013 11:00 AM - 12:30 PM
Session U7 CM.3 Transport Properties Grand Crescent - James Schilling, Washington University in St. Louis

11:00 AM U7.00001 Hydrostatic High-Pressure Studies to 25 GPa on the Model Superconducting Pnictide LaRu₂P₂

NEDA FOROOZANI, JINHYUK LIM, JAMES SCHILLING, Washington University in St. Louis, ROXANNA FOTOVAT, CHONG ZHENG, Northern Illinois University, ROALD HOFFMANN, Cornell University — Prior to the discovery of the Fe-pnictides in 2008, the ruthenium phosphate LaRu₂P₂ possessed the highest value of the superconducting transition temperature $T_c \approx 4$ K in the entire pnictide family. Recently, there has been renewed interest in this compound in an effort to understand why its $T_c$ value is as much as 15x lower than for some Fe-pnictides. Recent soft x-ray angle-resolved photoemission spectroscopy studies [1] have revealed that LaRu₂P₂ exhibits Fermi liquid behavior with weak electron-electron correlations. The superconducting properties of LaRu₂P₂ are also more isotropic than those of the Fe-pnictides. Unfortunately, the dependence of $T_c$ on hydrostatic pressure hasn’t yet been determined, although it is expected to have an emergent track record for uncovering valuable systematics and pointing the way to higher $T_c$ values. We report the first measurement for LaRu₂P₂ of the dependence of $T_c$ on hydrostatic pressure. In these studies a He-gas system provides pressures to 1 GPa followed by a He-loaded diamond-anvil cell to higher pressures. $T_c$ increases initially under pressure, but exhibits a relatively sharp downturn above 2 GPa, indicating a possible structural phase transition. The results of these studies are compared to related work on the Fe-pnictides. [1] Razzoli et al., Phys. Rev. Lett. 108, 257005 (2012).

1 Work at Washington Univ. supported by NSF grant DMR-1104742

11:15 AM U7.00002 A NiCrAl pressure cell up to 4.6 GPa and its application to cuprate and pnictide superconductors

NAOKI FUJIWARA, Kyoto University, YOSHIYA UWATOKO, University of Tokyo, TAKAHIKO MATSUMOTO, National Institute for Material Science — A NiCrAl-CuBe hybrid cell has been paid much attention because its maximum pressure goes beyond 3 GPa despite its large sample space. In the previous pressurizing trials for this pressure cell, we reached 4.0 GPa under a steady load of 15 ton. In the present trial, we have succeeded in reaching 4.6 GPa by using a short Teflon capsule as a pressure-mediation-liquid container. The pressure efficiency at 15 ton was 75%. The maximum expansion of the inner diameter of the NiCrAl cylinder was 5%, suggesting that 4.6 GPa is the upper limit of pressure. To keep high pressure above 4 GPa, a steady load control is needed: a pressure of 4.0 GPa under a steady load decreased to 3.7 GPa after the pressure cell was clamped and the steady load was released. The pressure cell is available to various experiments that need a large sample space. We have applied this pressure cell to nuclear magnetic resonance (NMR) measurements on cuprate and pnictide superconductors, such as $\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_7$, LaFeASO$_{1-x}$F$_x$, and CaFe$_{1-x}$Co$_x$AsF. These compounds have superconducting layers, and $T_S$ of these compounds are enhanced by pressure application. We review what happens at optimal pressure in electric and/or magnetic properties on a microscopic level.

1 Grant-in-Aid (Grant No. 23340101) from the Ministry of Education, Science and Culture, Japan

11:30 AM U7.00003 Effect of large uniaxial strain on carrier recombination mechanisms in GaAs

P. Grivickas, M.D. McCluskey, Y.M. Gupta, Washington State University — Carrier transport properties govern the operating characteristics of semiconductor devices. Strains are known to have a profound effect on carrier recombination processes, but details of these effects are not well understood due to the inherent limitations of common compression techniques. In this work, carrier lifetime measurements were obtained in shock-compressed GaAs using time- and spectrally-resolved photoluminescence measurements. Linear lifetime reduction was observed for different doping concentrations and for different crystal orientations. These experimental findings do not support previous hypothesis that emphasize recombination center formation in highly strained GaAs. A numerical carrier dynamics model, based on the continuity equation, was constructed to relate the experimental findings to the underlying material properties. It is shown that uniaxial strain primarily affects the non-radiative recombination mechanism and is consistent with the loss of quantum efficiency observed in GaAs. Work supported by DOE/NNSA.
11:45AM U7.00004 High temperature bulk diffusion in GaN, B. SADOVYI, I. GRZEGORY, J. WEYHER, I. DZIECIELEWSKI, A. KHACHAPURIDZE, S. POROWSKI, Institute of High Pressure Physics PAS, Sokolowska str., 29/37, 01-142 Warsaw, Poland, I. PETRUSHA, V. TURKEVICH, V. N. Bakul Inst. for Superhard Materials NASU, Avtozavodskaya str., 2, Kyiv, 04074, Ukraine, D. STATICHUK, V. N. Bakul Inst. for Superhard Materials NASU, Avtozavodskaya str., 2, Kyiv, 04074 UA, V. KAPUSTIANYK, Dep. of Phys., I. Franko National Univ. of Lviv, Dragomanova str., 50, Lviv UA 79005, M. ALBRECHT, Leibniz Inst. for Crystal Growth, Max-Born-Straße 2, 12489 Berlin, Germany, JHPF PAS TEAM, ISM NASU TEAM, LVIV I. FRANKO NATIONAL UNIV. COLLABORATION, IKZ COLLABORATION — Surprisingly, gallium nitride single crystals grown by High Nitrogen Pressure Solution method at temperature as high as 1750 K show non uniformities in distribution of impurities which suggests still slow bulk diffusion and very high melting temperature of GaN. In this work, GaN single crystals have been annealed at temperature up to 3350 K at pressure up to 9 GPa in order to induce homogeneization of crystal properties by bulk diffusion. For this purpose the crystals with intentional patterns of impurity distribution were used. The crystals became and after annealing were characterized by PL and CL mapping, photochemical etching sensitive to free electron concentration. It was established, that the bulk diffusion starts at temperature as high as 3300 K. It is reflected in uniformization of both optical and electrical properties of the crystals. This estimation suggests then melting temperature of GaN is significantly higher than current belief [1].


12:00PM U7.00005 Measurement and interpretation of shear viscosities at high pressures, EVAN ABRAMSON, Dept. of Earth and Space Sciences, University of Washington, Seattle, Washington — High pressures employed in the study of fluids allow density and temperature to be used as independent, experimental variables, providing extensive and clear comparison with theory. Measurements of the viscosities of simple fluids in the diamond-anvil cell have allowed confirmation of a hypothesized relation between viscosity and entropy, and a more general exploration of “isomorphs” as well as fluid-mixing rules. Densities and temperatures at which viscosities can be measured statically overlap those achievable by dynamic compression; inferences of viscosity from observations using, e.g., shock compression can thus be tested for accuracy.

Thursday, July 11, 2013 1:45PM - 3:00PM – Session V1 ME.3 Inelastic Deformation, Fracture, and Spall X Grand Ballroom III - Tommy Ao, Sandia National Laboratories

1:45PM V1.00001 Damage in Low Alloy Steel Produced by Sweeping, Interacting Detonation Waves, LAWRENCE HULL, GEORGE GRAY, JAMES FAULKNER, MATTHEW BRIGGS, Los Alamos National Laboratory — Detonation waves that sweep along the surface of a metal plate induce reduced pressure and enhanced shear, relative to the same detonation at normal incidence. Detonation waves at intermediate obliquity impress combined stress states. Release waves from the free surfaces may enter into play and contribute to the damage. Initiation of explosive at discrete points produces strong pressure, density, and velocity gradients in the gaseous explosive products where the waves collide that are impressed in an adjacent metal, causing similar stress gradients within the metal that often cause intense damage. In this work, we investigate damage generated in AISI 4130 steel by the combined effects of oblique drive and interacting detonation waves. The experimental data consists of multipoint velocimetry points probing the free surface in regions loaded by interacting detonation waves and regions between the interactions. Metallography on recovered plate records the plastic flow and damage correlated with the velocimetry data. Calculations provide further insight into the loading conditions created by the sweeping, interacting detonation waves. Span is indicated in most regions, but not some, and the alpha-epsilon strain-induced phase transformation appears in most regions, but not all. Correlations of the observed physical effects with incident wave obliquity and transverse position relative to the wave interactions are discussed.

2:00PM V1.00002 A Consistent Approach To Stochastic Seeding of Simulations of Fragmenting Ductile Metals.1, MATTHEW BARHAM, JAMES STÖLKEN, MUKUL KUMAR, Lawrence Livermore National Laboratory — For failure by brittle fracture the well-known weakest-link arguments have led to widespread use of a two-parameter Weibull distribution. The probability of failure by a ductile damage mechanism at small plastic strains is exceedingly small. This results in a threshold for deformation induced damage and attendant failure that should be manifest in the statistical description. A three-parameter Weibull distribution with a lower cut-off satisfies this constraint. The three-parameters are determined systematically from experiments. The Weibull modulus is estimated by examining the results of scaled experiments. The values of the most-likely failure strain were inferred from simulations of quasi-static tests. The lower cut-off failure strain was estimated from the tensile test data. This approach was applied to different microstructures of AISI 4340 steel achieved through various heat treatments to determine the three parameters and constitutive response for each heat treatment. Exploding pipe simulations were run to determine fragment distributions for two explosives and each heat treatment. These simulated distributions were then compared to high fidelity experimental data for distributions of the same heat treatments and explosives simulated.

1Prepared by LLNL under Contract DE-AC52-07NA27344.

2:15PM V1.00003 ABSTRACT WITHDRAWN —

2:30PM V1.00004 2169 Steel Waveform Experiments, M.D. FURNISH, C.S. ALEXANDER, W.D. REINHART, J.L. BROWN, Sandia National Laboratories — In support of efforts to develop multiscale models of materials, we performed eight gas gun impact experiments on 2169 steel (21% Cr, 6% Ni, 9% Mn). These experiments provided shock, reshock and release velocimetry data, with initial shock stresses ranging from 10 to 50 GPa (particle velocities from 0.25 to 1.05 km/s). Both windowed and free-surface measurements were used, with samples 1 to 5 mm thick. The study focused on dynamic strength determination via the release/reshock paths. Reshock tests with explosively welded impactors produced clean results. The free-surface samples, which were steps on a single piece of steel, showed lower wavespeeds for thin (1 mm) samples than for thicker (2 or 4 mm) samples. A configuration on dynamic strength determination via the release/reshock paths. Reshock tests with explosively welded impactors produced clean results. The free-surface samples, which were steps on a single piece of steel, showed lower wavespeeds for thin (1 mm) samples than for thicker (2 or 4 mm) samples. A configuration

2:45PM V1.00005 Dynamic Crack Tip Opening Displacement (DCTOD) as governing parameter for materials fragmentation, NICOLA BONORA, ANDREW RUGGIERO, GABRIEL TESTA, University of Cassino and Southern Lazio, GIANLUCA IANNITTI, Techdyn Engineering, DOMENICO GENTILE, University of Cassino and Southern Lazio — Fragmentation in metals can be approached either by Mott statistical or by Energy-based fragmentation theory. Recently, Grady showed that the two theories can be reconciled showing that the material parameter that drives tendency to fragmentation and fragment size is the dynamic fracture toughness. Experimental data do not completely agree with these conclusions. In this paper, the dynamic CTOD – crack tip opening displacement – is proposed as fracture parameter which can account for plastic deformation occurring prior fracture. Here, an experimental procedure for determining the DCTOD is presented. Two sample geometries, namely 1/2” compact tension C(T) and circumferential crack bar tension ECCB(T), have been investigated for their use with tensile Hopkinson bar testing equipment. The respective calibration functions in the dynamic range were determined via FE. DCTOD was measured using both high speed video recording with digital image correlation (DIC) technique and clip gauge at the crack mouth. The proposed procedure has been used to investigate dynamic fracture resistance of 316L stainless steel and high purity copper (99.98%) and to correlate with available fragmentation data.
We propose some physics rich experiments to better understand the dynamics of this element utilizing the best experimental data and theoretical calculations. The equilibrium EOS includes the GeI (diamond), GeII (beta-Sn) and liquid phases. We will findings related to the stability of the high pressure rhombohedral phase of the pure vanadium and the equation of state, and the influence of the alloying on x-ray diffraction experiments in diamond anvil cell of pure vanadium and V-Ti alloys at ambient temperature up to 220 GPa. In this paper we will discuss our transition has also been reported from point loading (indentation) experiments. Particularly pure amorphous Ge as starting material can be reliably phase 1:45PM V2.00001 Phase Diagram of Sn into the Megabar Pressure Range, RICHARD BRIGGS, The University of Edinburgh, ASHKAN SALAMAT, Harvard University, DOMINIK DAISENBERGER, Diamond Light Source, PIERRE-BOUVIER, CNRS, SYLVAIN PETITGIRARD, GASTON GARBARINO, European Synchrotron Radiation Facility, AGNES DEWAELLE, CEA, PAUL McMILLAN, University College London — The melting curve of Sn has previously been studied using shock techniques up to P ~ 50 GPa, and recent diamond anvil cell experiments showed flat melting temperatures between 40 and 68 GPa. We performed new melting experiments using laser-heated diamond anvil cell techniques combined with in situ synchrotron X-ray diffraction, revealing a steep rise in melting slope above 70 GPa up to a maximum Tm ~5500 ± 500 K at 1.05 Mbar. Those results immediately paved the way for laser driven shock experiments that could probe both the melting relation following shock compression and the solidus below the melting curve in the 1-10 Mbar pressure range via ramp compression and diffraction techniques. We also performed room temperature experiments to 1.4 Mbar using the diamond anvil cell with near hydrostatic conditions (He loadings) and synchrotron X-ray diffraction. Our results at room temperature reveal a previously unreported distortion of the body centered tetragonal phase (14/mmm) to an orthorhombic structure (Immm) at 32 GPa. Between 40 and 70 GPa, the X-ray diffraction patterns reveal two structures that can be assigned to this body centered orthorhombic structure and the second to the previously reported bcc (Im-3m) phase. The phase diagram spreading across 2 Mbar and 6000 K will be discussed. 2:00PM V2.00002 Sound velocity under shock compression and bct-bcc transition of Ti1, HAI FENG LIU2, IAPCM, LIN ZHANG3, IFP, GONGMU ZHANG, HAI FENG SONG, IAPCM, XUEMEI LI, IFP, YAN HONG ZHAO, IAPCM, JIANBO HU, IFP, TANG LI, IAPCM, IAPCM TEAM, IFP TEAM — The longitudinal sound velocity of material can be resolved from the particle velocity of window profile under shock loading. Two analysis methods are proposed. One is name for the speed change derivative of sound velocity versus time and the other is the continue lowering of velocity plateau. We carefully analysis the experimental data from the direct reverse-impact configuration and the new sound velocity data are provided. The results show the experimental points of the longitudinal sound velocity against shock pressure are dispersive and the range of transition pressure from bct-bcc under dynamic compression is difficult to obtain. 1This research is supported by the Science and Technology Development Foundation of Chinese Academy of Engineering Physics under Grant No. 2009A0101004 2Data Center of High Energy Density Physics, Institute of Applied Physics and Computational Mathematics(IAPCM) 3Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics(IFP) 2:15PM V2.00003 Powder diffraction from solids in the terapascal regime, J. RYAN RYGG, LLNL — A method of obtaining powder diffraction data on dynamically-compressed solids has been implemented at the Jupiter and OMGEGA laser facilities. Thin powdered samples are sandwiched between diamond plates, and ramp compressed in the solid phase using a gradual increase in the drive-laser intensity. The pressure history in the sample is determined by back-propagation of the measured diamond free-surface velocity. A pulse of x-rays is produced at the time of peak pressure by laser illumination of a thin Cu or Fe foil, and collimated at the sample plane by a pinhole cut in a Ta substrate. The diffracted signal is recorded on x-ray sensitive material, with a typical d-spacing uncertainty of approximately 0.01 Å. This diagnostic has been used up to 1.2 TPa (12 Mbar) to verify the solidity, measure the density, constrain the crystal structure, and evaluate the strain-induced texturing of a variety of compressed samples spanning atomic numbers from 6 (carbon) to 82 (lead). 2:45PM V2.00004 A new polymorph of germanium, BIANCA HABERL, Australian National University, Australia, MALCOLM GUTHRIE, Geophysical Laboratory, Carnegie Institution of Washington, USA, BRETT C. JOHNSON, University of Melbourne, Australia, GUOYIN SHEN, HP-CAT, Geophysical Laboratory, Carnegie Institution of Washington, USA, BRAD D. MALONE, Harvard University, USA, MARVIN L. COHEN, University of California-Berkeley, USA and Lawrence Berkeley National Laboratory, USA, JIM S. WILLIAMS, JODIE E. BRADBY, Australian National University, Australia — The behavior of germanium under high pressure has been studied for many decades using diamond-anvil cells (DACs). A series of metal-metal transitions has been observed after the initial transition to the metallic β-Sn structure at ~10 GPa. More recently, evidence for the semiconductor-metal transition has also been reported from point loading (indentation) experiments. Particularly pure amorphous Ge as starting material can be reliably phase transformed. These transitions are not reversible however, and meta-stable crystalline phases can be recovered upon pressure release. In this study we report experimental evidence from both point loading and in-situ DAC experiments for a new polymorph of Ge with the θ structure, the same as observed for silicon. In the point loading case, the final phases after unloading are characterized using Raman spectroscopy in conjunction with computations employing density functional theory. In the DAC case, in-situ X-ray diffraction using synchrotron radiation was employed. This combination of two such very different methods for pressure application yields a more comprehensive picture of the phase behavior of Ge. 3:00PM V2.00005 Germanium Multiphase Equation of State, SCOTT CROCKETT, JOEL KRESS, SVEN RUDIN, GIULIA DE LORENZI-VENNERI, Los Alamos National Laboratory — A new SESAME multiphase Germanium equation of state (EOS) has been developed utilizing the best experimental data and theoretical calculations. The equilibrium EOS includes the Gel (diamond), Gell (beta-Sn) and liquid phases. We will also explore the meta-stable Gell (tetragonal) phase of germanium. The theoretical calculations used in constraining the EOS are based on quantum molecular dynamics and density functional theory phonon calculations. We propose some physics rich experiments to better understand the dynamics of this element. 3:15PM V2.00006 Phase Stability and Equation of State of Vanadium and V-Ti alloys to 220 GPa1, ZSOLT JE NEI, HYUN CHAE CYN, WILLIAM J. EVANS, Lawrence Livermore National Laboratory, SIMON MACLEOD, Atomic Weapons Establishment, UK, STANISLAV SINOGIEKIN, YUE MENG, HPCAT — Experimental studies of vanadium found that during compression it undergoes a phase transition from the low pressure body centered cubic crystal structure to a rhombohedral phase at 65 GPa when compressed under quasihydrostatic conditions and as low as 30 GPa under uniaxial compression (PRB 83, 054101). Theoretical studies are in reasonable agreement with the transition pressure and predict that upon further compression above 200 GPa the bcc phase becomes stable again. The latest study (PRL 103, 235501) predicts that alloying vanadium with Ti-Ti alloys at ambient temperature up to 220 GPa. In this paper we will discuss our findings related to the stability of the high pressure rhombohedral phase of the pure vanadium and the equation of state, and the influence of the alloying on the EOS. 1This work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. HPCAT use is supported by DOE-BES, DOE-NSNSA, NSF, and the W.M. Keck Foundation. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.
3:30PM V2.00007 Embedded atom model for tin and MD simulation of shock loading and melting. FILIPP SAPIPOZHNIKOV, GENNADY IONOV, VLADIMIR DREMOV, RFNC-VNIITF, Snezhinsk, Russia, LAURENT SOULARD, CEA/DAM, France — The goal of the work was to develop an interatomic potential, that can be used in large-scale classical MD simulations to predict tin properties near the melting curve, the melting curve itself, and the kinetics of melting and solidification when shock and ramp loading. According to phase diagram, shocked tin melts from bcc-phase, and since the main objective was to investigate melting, the EAM was parameterized for bcc-phase. The EAM was optimized using isothermal compression data (experimental at T=300K and ab initio at T=0K for bcc, fcc, bct structures), experimental and QMD data on the Hugoniot and on the melting at elevated pressure. The Hugoniot calculation centered at $\beta$-tin at ambient conditions showed that the calculated Hugoniot is in good agreement with the results of experimental and QMD data above $\beta$-BCT transition pressure. A series of calculations of overcooled liquid in pressure range corresponding to bcc-phase showed crystallization into bcc-phase. Since the principal Hugoniot of tin originates from the $\beta$-tin that is not described by this EAM the special initial state of bcc samples was constructed to perform large-scale MD simulations of shock loading.

Thursday, July 11, 2013 1:45PM - 3:45PM
Session V3 NT.1 Novel Techniques: Diamond Anvil Cells II
Fifth Avenue - Jon Eggert, Lawrence Livermore National Laboratory

1:45PM V3.00001 Confocal microscopy of fluids under static pressure, MATTHEW MCCULLOUGH, Washington State University — There are few reliable methods for obtaining equations of state for fluids under static pressure. We are developing confocal microscopy to investigate fluids in a diamond-anvil cell. Unlike conventional optical microscopy, confocal microscopes collect data point-by-point, enabling three-dimensional image reconstruction. By combining these images with Fabry-Perot interference measurements, we determine the volume and refractive index, as a function of pressure, in the same experiment.

2:00PM V3.00002 Pressure Generation Using Micro Size Nano-Polycrystalline Diamond Anvil, TAKEHIKO YAGI, TAKESHI SAKAI, TETSUO IRIFUNE, GRC, Ehime University, YUYA SUZUKI, YASUSHI KURODA, Hitachi High-Technologies Corporation — Since the first report of static high-pressure generation above mega bar using diamond anvil (Mao and Bell, 1978), further extension of pressure range was achieved mainly by the reduction of cutlet size. Nowadays it become possible to do experiments at the condition corresponding to the center of the Earth, that is above 350 GPa, using diamond anvils with a cutlet size of less than 50 microns. Dubrovinsky et al. (2012) reported a generation of pressure above 600 GPa using micro-ball nanodiamond anvils, which were synthesized from grassy carbon in the multi-anvil high-pressure and high-temperature apparatus. Here we report the trial to achieve very high pressures using micro size nano-polycrystalline diamond anvils, which were fabricated using Focused Ion Beam (FIB) technique. This technique allows generation of 100um micro-diamond anvils with a cutlet size of 0.3 microns precisely from the nano-polycrystalline diamond, which was invented at Ehime University, and is believed to be one of the hardest materials so far known. The micro-anvils were placed at the center of ordinary diamond anvils with a cutlet size of 300 micron and compressed in the pressure transmitting media which applies confining pressure to the micro-anvils. The detail of experiments will be reported.

2:15PM V3.00003 Measuring the structure factor of simple fluids under extreme conditions, GUNNAR WECK, CEA, DAM, DIF, Bruyères-le-Châtel, 91297 Arpajon Cedex, France — The structure and dynamics of fluids, although a long standing matter of investigations, is still far from being well established. In particular, with the existence of a first order liquid-liquid phase transition (LLT) discovered in liquid phosphorus at 0.9 GPa and 1300 K [1] it is now recognized that the fluid state could present complex structural changes. At present, very few examples of LLTs have been clearly evidenced, which may mean that a larger range of densities must be probed. First order transitions between a molecular and a polymeric liquid have been recently predicted by first principles calculations in liquid nitrogen at 88 GPa and 2000 K [2] and in liquid CO$_2$ at 45 GPa and 1850 K [3]. The only device capable of reaching these extreme conditions is the diamond anvil cell (DAC), in which, the sample is sandwiched between two diamond anvils of thickness 100 times larger. Consequently, the diffracted signal from the sample is very weak compared to the Compton signal of the anvils, and becomes hardly measurable for pressures above ~20 GPa. A similar problem has been faced by the high pressure community using large volume press so as to drastically reduce the x-ray background from the sample environment. In the angle-dispersive diffraction configuration, it was proposed to use a multichannel collimator (MCC) [4]. This solution has been implemented to fit the constraints of the Paris-Edinburgh (PE) large volume press and it is now routinely used on beamline ID27 of the European Synchrotron Radiation Facility [5,6]. In this contribution, we present our adaptation of the MCC device accessible at ID27 for the DAC experiment. Because of the small sample volume a careful alignment procedure between the MCC slits and the DAC had to be implemented. The data analysis procedure initially developed by Eggert et al. [7] has also been completed in order to take into account the complex contribution of the MCC slits. A large reduction of the Compton diffusion from the diamond anvils is obtained enabling quantitative structure factor measurement, even for the weakest x-ray scatterer liquid. Experimental results on fluid hydrogen will be presented to test the limits of this new setup. In collaboration with Gaston Garbarino, ESRF, France; Frederic Datchi, Sandra Ninet, Université Pierre et Marie Curie-Paris VI, France; Dylan Spaulding, Paul Loubeyre, CEA, DAM, DIF, France; and Mohamed Mezouar, ESRF, France.

References:

2:45PM V3.00004 ABSTRACT WITHDRAWN —

3:00PM V3.00005 High pressure magnetic measurements on strongly correlated electron systems with miniature ceramic anvil high pressure cell. NAOYUKI TATEIWA, YOSHINORI HAGA, TATSUMA MATSUEDA, ETSUJI YAMAMOTO, Advanced Science Research Center, Japan Atomic Energy Agency, ZACHARY FISK, University of California — We have designed a miniature ceramic anvil high pressure cell (mCAC) for magnetic measurements at pressures up to 12.6 GPa in a commercial superconducting quantum interference (SQUID) magnetometer [N. Tateiwa et al., Rev. Sci. Instrum. 82, 053906 (2011)., ibid. 83, 053906 (2012)]. The simplified mCAC without anvil alignment mechanism is easy-to-use for researchers who are not familiar with high-pressure technology. The production cost is about one tenth of that of the diamond anvil cell (DAC). Recently, the background magnetization in the mCAC was significantly reduced, enabling more precise magnetic measurements at low temperatures. In this conference, we will show our recent modifications in the mCAC and experimental results on rare earth compound Yb$_2$Cu$_3$Si$_2$. Yb$_2$Cu$_3$Si$_2$ is a paramagnetic compound at ambient pressure. The pressure-induced phase has been suggested above 8 GPa by previous studies with the ac magnetic susceptibility and the heat capacity measurements. We confirm the spontaneous dc magnetization in the pressure-induced ferromagnetic phase of the dc magnetic measurement. We have studied the anisotropy in the magnetic property in the pressure-induced phase around 11 GPa and found that the phase has the strong Ising-type uniaxial anisotropy.

References:
3:15PM V3.00006 Designer Diamonds: Applications in Iron-based Superconductors and Lanthanides

YOGESH VOHRA, Department of Physics, University of Alabama at Birmingham (UAB) — This talk will focus on the recent progress in the fabrication of designer diamond anvils as well as scientific applications of these diamonds in static high pressure research. The two critical parameters that have emerged in the microwave plasma chemical vapor deposition of designer diamond anvils are (1) the precise [100] alignment of the starting diamond substrate and (2) balancing the competing roles of parts per million levels of nitrogen and oxygen in the diamond growth plasma. The control of these parameters results in the fabrication of high quality designer diamonds with culet size in excess of 300 microns in diameter. The three different applications of designer diamond anvils will be discussed (1) simultaneous electrical resistance and crystal structure measurements using a synchrotron source on Iron-based superconductors with data on both chemically and hole doped BaFe2AS2 materials and other novel superconducting materials (2) high pressure high-temperature melting studies on metals using eight-probe Ohmic heating designer diamonds and (3) high pressure low temperature studies on magnetic behavior of 4f-lanthanide metals using four-probe electrical resistance measurements and complementary neutron diffraction studies on a spallation neutron source. Future opportunities in boron-doped conducting designer diamond anvils as well as fabrication of two-stage designer diamonds for ultra high pressure experiments will also be presented.

This work was supported by the Department of Energy (DOE) - National Nuclear Security Administration (NNSA) under Grant No. DE-FG52-10NA26060.

Thursday, July 11, 2013 1:45PM - 3:30PM –
Session V4 NM.2 Nanomaterials
Vashon - Takahiro Matsuoka, Osaka University

1:45PM V4.00001 Shock-Induced Nanostructure Formation in Copper
YURI MESHCHERIAKOV, NATALIA ZHIGACHEVA, ALEXANDRE DIVAKOV, GRIGORII KONOVALOV, Institute of Problems of Mechanical Engineering RAS, Saint-Petersburg, Russia, BORIS BARAKHTIN, CentralResearch Institute of Constructional Materials "Prometei" — Shock-induced nanostructure in polycrystalline copper of varied purity is found to be nucleated within narrow range of strain rates $5 \cdot 10^6$ to $5.7 \cdot 10^6$ s$^{-1}$. Shock loading of plane targets was conducted in two ways. The first way allows interference of longitudinal and lateral release waves whereas in the second configuration the studied material was conically pressed inside the copper disks, which allows to avoid a passage of lateral waves through the material of interest. The chaotically distributed within grains 3D-nanostructure formations of 15 $\mu$m in diameter are the result of dynamic response of material on combined loading with longitudinal and lateral release waves, which can be provided only in the first way of shock loading i.e. under 3D conditions. The formations consist of 3D-network of mutual perpendicular microtwins of 100-200 nm spacing. Energy and momentum expended on formation of the structures is shown to be quantitatively characterized by “defect of particle velocity” – difference between impact velocity under symmetrical collision and free surface velocity. There is a threshold strain rate at which defect of particle velocity begins to grow very fast, dimension of formations increases, and simultaneously hardness and spall-strength of material grow as well.

2:00PM V4.00002 High-Pressure Nanocrystals: New Structure and New Phase Transition Sequence
BO ZOU, State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China — High-pressure studies offer a potential strategy to the synthesis of nanocrystals with new phases, and provide new insights into the phase stability in metastable NCs. We have studied the stability of metastable ZB- and WZ-MnS NCs under high pressure and found ZB-nanoparticles and ZB/WZ-nanobipods are stable below 5.3 and 2.9 GPa, respectively. With further compression, all these metastable MnS NCs directly convert to the stable RS-MnS. The WZ-CuGaS$_2$ nanocrystals undergo a transition to another disordered RS phase above 15.9 GPa, which is stable up to 30.3 GPa. Upon release of pressure, the sample was irreversible and intriguingly converted into the energetically more favorable and ordered Chalcopryite (CH) structure. The YPO$_4$ nanoparticles exhibit a distinct transition sequence: zinc to scheelite phase ($\sim$18 GPa) without the metastable monazite phase. Additionally, this transition sequence was investigated on the YV$_{1-x}$P$_x$O$_4$ nanoparticles. The transition pressure is reduced with more VO$_2$ substituting for PO$_4$ units.

1This work is supported by NSFC (91227202) and RFPD (2012006130006).

2:15PM V4.00003 Molecular monolayers under high pressure: a study using surface enhanced Raman scattering and vibrational sum frequency generation spectroscopy
YUANXI FU, DANA DLOTT, School of Chemical Sciences, University of Illinois at Urbana-Champaign — Vibrational spectra of molecular monolayers in a diamond anvil cell (DAC) reveal the conformation and packing state of the monolayers undergoing large-amplitude deformations. Measuring monolayer spectra under high pressure can be difficult due to the small number of molecules. We used surface enhanced Raman scattering (SERS) and vibrational sum frequency generation (VSFG) spectroscopy in a DAC to address the challenge. Localized surface plasmon resonance generated on curved metal surfaces enhances the adsorbates’ Raman scattering (SERS) and vibrational sum frequency generation (VSFG) spectroscopy cross-sections by factors of $10^3$, allowing SERS spectra of monolayers formed by organic thiols on silver coated polystyrene nanospheres and dyes on silver colloidal nanoparticles to be studied up to several GPa. To better understand the role of curvature, monolayers on planar surfaces were studied using a new diamond anvil cell for VSFG spectroscopy. VSFG is a nonlinear coherent vibrational spectroscopy that uses converging IR and visible femtosecond laser pulses. The VSFG spectra of long-chain alkane monolayers were studied up to several GPa.

2:30PM V4.00004 Characterization of Elastic and Vibrational Properties of Dense BC$_x$ Nano-Phases Synthesized under High-Pressure and High-Temperature
JIA, ERIC HALEBRAND, TAYRO ACOSTA, LI-CHUNG MING, University of Hawaii — We use Raman scattering to study cold press phase transitions in the graphitic $\beta$-BC$_x$ phase and graphite under high pressure up to 84 GPa. It is shown that the E$_{2g}$ Raman active mode of graphite (Gpeak) can be detected up to 84 GPa. We demonstrate that (a) there is a phase transition in graphite and in $\gamma$-BC$_x$ at 35 GPa and (b) above 35 GPa the graphite and $\gamma$-BC$_x$ transform in a high pressure phase, fully sp$^3$ bonded $\alpha$-BC$_x$ phases. Below the phase transition a polynomial fit to the G peak position versus pressure data yielded the following quadratic relation; above 35 GPa it exhibits linear behavior for graphite as well as for $\gamma$-BC$_x$ phase. A direct transformation of graphitic phases in the BC$_x$ system with high concentration of boron (1.5 $< x < 8$) under high pressure and high temperature was studied. It was found that graphitic phases transform to new cubic BC$_x$($c$-BC$_3$, $c$-B$_2$C$_3$) phases in a diamond anvil cell (DAC) at high temperature, 2200 K, and high pressure, 31 GPa. The atomic structure, bonding between atoms, and nanostructure was determined using transmission electron microscopy (TEM), x-ray diffraction and transmission electron microscopy-electron energy-loss spectroscopy (EELS). Elastic properties of the BC$_x$ phases were determined by Laser Ultrasonic and Brillouin scattering techniques.

3This work was supported by the U.S. Department of Energy Grant NO. DE-FG02-07ER46408.
2:45PM V4.00005 Extreme synthesis and characterization of an ultrananocrystalline diamond aerogel in a diamond anvil cell. PETER PAUZAUSKIE, University of Washington — High-surface-area mesostructured carbon materials have attracted a great amount of attention in recent years because of a growing number of applications in energy storage, chemical catalysis, separations, and sensing. In particular, amorphous carbon aerogels have attracted much interest since the 1980’s due to their low density, large intrinsic surface areas (>1000 m²/g), large pore volume, low dielectric constant, and high strength. In this talk we present the use of high-pressure (>20 GPa) laser-heating (>1500°C) within a diamond anvil cell (DAC) to convert the amorphous network of a low-density (40 mg/cc) carbon aerogel into an ultrananocrystalline diamond aerogel. Raman spectroscopy is used to probe the amorphous-to-diamond phase transition at pressure within the DAC. High-resolution transmission electron microscopy images of recovered material indicate diamond crystallite sizes range from 1 to 100 nm, with electron diffraction and electron energy loss confirming the presence of the diamond phase. Photoluminescence spectroscopy and confocal time-correlated single-photon counting indicate the recovered material contains both negatively-charged and neutral nitrogen-vacancy (NV) complexes. Synchrotron scanning transmission x-ray microscopy (STXM) is used to compare the carbon electronic density-of-states of the amorphous starting material with the recovered diamond aerogel with <100 meV energy resolution. Finally, we use nanoscale secondary ion mass spectrometry to investigate doping of the resorcinol-formaldehyde starting material with the aim of chemically tuning heteroatomic point defects within this diamond material system.

3:15PM V4.00006 Morphology-Tuned Phase Transitions of Anatase TiO₂ Nanowires under High Pressure. QUANJUN LI, BENYUAN CHENG, XUE YANG, RAN LIU, BO LIU, Jili University, JING LIU, Institute of High Energy Physics, Chinese Academy of Sciences, ZHIQIANG CHEN, GeoScience Department, Stony Brook University, BO ZOU, TIAN CUI, BINGBING LIU, Jili University — The phase transitions of one-dimensional (1D) anatase TiO₂ nanowires were studied by in situ high pressure synchrotron X-ray diffraction (XRD) and Raman scattering. A direct anatase-to-baddeleyite transformation was observed at ~9 GPa, which is clearly different from the size-dependent phase transition behaviors for nanocrystalline TiO₂. We found the higher compressibility in the c-axis compared to the a-axis for anatase nanowires which may be attributed to both the crystal structural feature and the growth direction of the nanowires. This phase transition of the TiO₂ nanowires shows obvious morphology-tuned behaviors. Upon decompression, the baddeleyite phase transformed into α-PbO₂ phase. The morphology of the TiO₂ nanowires shows excellent stability and TiO₂ nanowires with α-PbO₂ phase were obtained at ambient conditions through a compression-decompression cycle. These results indicate that the nanoscale quasi-1D structure of TiO₂ nanowires may contribute to the high pressure phase transitions showing unique morphology-tuned behaviors.

Thursday, July 11, 2013 1:45PM - 3:30PM –
Session V5 LS Large Scale Experiments II Cascade I - Russ Olson, Los Alamos National Laboratory

1:45PM V5.00001 Simultaneous unfolding of compression and opacity from time-resolved radiography¹. D.C. SWIFT, J.A. HAWRELIAK, Lawrence Livermore National Laboratory, S.D. ROTHMAN, AWE Aldermaston, A. KRITCHER, T. DOEPPNER, G.W. COLLINS, Lawrence Livermore National Laboratory, J. GAFFNEY, S. ROSE, Imperial College — Radiographs of symmetric objects can be analyzed to give the spatial variation of attenuation, as in the Abel inversion of an axisymmetric object. If the opacity is known, the mass density can be derived from the attenuation. The space- and time-variation of density is needed to make equation of state (EOS) measurements by radiography, e.g. by measuring the speed and compression of a shock. However, in our experiments using hohlraum drive at the National Ignition Facility (NIF) to perform EOS measurements at gigabar pressures with spherically-converging shocks, the opacity may vary by an order of magnitude because of ionization. We have developed a new algorithm to simultaneously deduce the compression and opacity of the sample given time-resolved radiographs with a Lagrangian location behind the shock, such as the edge of the sample. This approach relies on spatial integration to deduce the opacity in the region just behind the shock from the difference between the known and apparent mass. We assume that the change in opacity is dominated by shock-heating, so that subsequent variations, as shocked material is either released or compressed further, are negligible or can be accounted for by a model. We used this algorithm to analyze our NIF data on the Hugoniots of CH at 10-40 TPa.

¹This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

2:00PM V5.00002 Analysis of data from shockless compression experiments to multi-megabar pressure¹. JEAN-PAUL DAVIS, JUSTIN BROWN, RAYMOND LEMKE, MATTHEW MARTIN, MARCUS KNUDSON, Sandia National Laboratories — Quasi-isentropic, shockless ramp-wave experiments promise accurate equation-of-state (EOS) data in the solid phase at relatively low temperatures and multi-megabar pressures. In this range of pressure, isothermal diamond-anvil techniques have limited pressure accuracy due to reliance on theoretical EOS of calibration standards, thus accurate quasi-isentropic compression data would help immensely in constraining EOS models. Multi-megabar shockless compression experiments using the Z Machine at Sandia as a magnetic drive with stripline targets have been performed on a number of solids. New developments will be presented in the analysis of data from these experiments using the single-sample inverse Lagrangian approach, including topics such as 2-D and magneto-hydrodynamic (MHD) effects and uncertainty quantification. Results will be presented for selected metals, with comparisons to independently developed EOS.

¹Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

2:15PM V5.00003 Ramp compression of a metallic liner driven by a shaped 5 MA current on the SPHINX machine. THIERRY D’ALMEIDA, FRANCIS LASSALLE, ALAIN MORELL, JULIEN GRUNENWALD, FRÉDÉRIC ZUCCHINI, ARNAUD LOYEN, CEA, THOMAS MAYSOUNNAVE, ITHPP, ALEXANDRE CHUVATIN, Ecole Polytechnique — SPHINX is a 6MA, 1-µs Linear Transformer Driver operated by the CEA Gramat (France) and primarily used for impinging Z-pinch loads for radiation effects studies. Among the options that are currently being considered for improving the generator performances, there is a compact Dynamic Load Current Amplifier (DLCM). A method for performing magnetic ramp compression experiments, without modifying the generator operation scheme, was developed using the DLCM to shape the initial current pulse. We present the overall experimental configuration chosen for these experiments, based on electrical and hydrodynamic simulations. Initial results obtained over a set of experiments on an aluminum cylindrical liner, ramp-compressed to a peak pressure of 23 GPa, are presented. Details of the electrical and Photonic Doppler Velocimetry (PDV) setups used to monitor and diagnose the ramp compression experiments are provided. Current profiles measured at various locations across the system, particularly the load current, agree with simulated current profile and demonstrate adequate pulse shaping by the DLCM. The liner inner free surface velocity measurements agree with the hydrocode results obtained using the measured load current as the input. Higher ramp pressure levels are foreseen in future experiments with an improved DLCM system.
single crystals, 0.2 mm to 3 mm thick, were shock loaded along the two axes, a, Joint Institute for High Temperatures of RAS, Moscow, 125412 Russia, A. SAVINYKH, S. RAZORENOV, Institute of Problems of Chemical Physics of RAS, G. GARKUSHIN, Institute of Problems of Chemical Physics of RAS, Chernogolovka, 142432 Russia, G. KANEL, and elevated temperatures

The crystals demonstrate the largest spall strength at shock loading along the -orientation the growth is caused by decrease of elastic constants and not with an increase of resolved shear stress along the pyramidal slip planes. In the other orientations the resolved shear stresses in slip planes at the HEL increased with temperature. At inclined, off-axis direction and is associated with smallest HEL value. For all orientations, we observed elastic precursor decay and growth of the HEL values at which sub-granular physical processes and inter-granular organization couple to determine microstructure, crucially impacting constitutive response at the engineering macroscale. For these reasons Los Alamos is proposing the MaRIE facility as a National User Facility to meet this need. In particular, three key science challenges will be identified: Link material microstructure to macroscopic behavior under dynamic deformation conditions; Make the transition from observation and validation to prediction and control of dynamic processes; and Develop the next generation of diagnostics, dynamic drivers, and predictive models to enable the necessary, transformative research.

Thursday, July 11, 2013 1:45PM - 3:45PM – Session V6 ME.4 Strength VII Cascade II - Curt Bronkhorst, Los Alamos National Laboratory

1:45PM V6.00001 Response of magnesium single crystals to shock-wave loading at normal and elevated temperatures, G. GARKUSHIN, Institute of Problems of Chemical Physics of RAS, Chernogolovka, 142432 Russia, G. KANEL, Joint Institute for High Temperatures of RAS, Moscow, 125412 Russia, A. SAVINYKH, S. RAZORENOV, Institute of Problems of Chemical Physics of RAS, Chernogolovka, 142432 Russia, D. JONES, W. PROUD, Institute of Shock Physics, Imperial College London, London, SWT 2AZ, United Kingdom — Magnesium single crystals, 0.2 mm to 3 mm thick, were shock loaded along the two axes, a, c and the direction at 45 degrees to the c-axis. At the room temperature the response is very similar to that observed by Pope and Johnson for beryllium single crystals (1974). Shock compression along the c-axis causes inelastic deformation by means of pyramidal slip and twinning and is associated with the largest HEL. The easiest basal slip was activated by shock loading along the inclined, off-axis direction and is associated with smallest HEL value. For all orientations, we observed elastic precursor decay and growth of the HEL values with increasing temperature. However, for the c-orientation the growth is caused by decrease of elastic constants and not with an increase of resolved shear stress along the pyramidal slip planes. In the other orientations the resolved shear stresses in slip planes at the HEL increased with temperature. At inclined shock compression we found two plastic shock waves for which the stress behind the first depends on the peak stress associated with the second plastic wave.

2:00PM V6.00002 High strain rate behavior of pure metals at elevated temperature, GABRIEL TESTA, NICOLA BONORA, ANDREW RUGGIERO, University of Cassino and Southern Lazio, GIANLUCA IANNITTI, Techdyn Engineering, GENTILE DOMENICO, University of Cassino and Southern Lazio — In many applications and technology processes, such as stamping, forging, hot working etc., metals and alloys are subjected to elevated temperature and high strain rate deformation process. Characterization tests, such as quasistatic and dynamic tension or compression test, and validation tests, such as Taylor impact and DTE - dynamic tensile extrusion -, provide the experimental base of data for constitutive model validation and material parameters identification. Testing material at high strain rate and temperature requires dedicated equipment. In this work, both tensile Hopkinson bar and light gas gun where modified in order to allow material testing under sample controlled temperature conditions. Dynamic tension tests and Taylor impact tests, at different temperatures, on high purity copper (99.98%), tungsten (99.95%) and 316L stainless steel were performed. The accuracy of several constitutive models (Johnson and Cook, Zerilli-Armstrong, etc.) in predicting the observed material response was verified by means of extensive finite element analysis (FEA).

2:15PM V6.00003 Effects of sample temperature on spall fracture in laser shock-loaded metals between about 30 K and 1000 K, THIBAUT DE RESSEGUIER, Institut P´ - UPR CNRS 3346 - ENSMA, EMILLEN LESCOTTE, CEA, DAM, DIF, GCI, Argonne, France. DIDIER LOISON, Institut P´ - UPR CNRS 3346 - ENSMA, JEAN-MARC CHEVALIER, CEA, CESTA, 33114 Le Barp Cedex, France, INSTITUT P´ - DPMM TEAM, CEA - DAM - DIF TEAM, CEA - CESTA TEAM — For many years, spall fracture of shock-loaded materials has been one of the most widely studied phenomena in shock physics, for both basic and technological motivations. Laser driven shocks provide a means to investigate this process over ranges of extremely high strain rates and short durations, and they allow recovering spalled samples more easily than impact or explosive loading techniques. In this paper, we present laser shock experiments on gold, aluminium and iron, over a wide range of initial temperatures from cryogenic conditions (relevant in the context of inertial confinement fusion) to about 1000 K. Time-resolved measurements of the free surface velocity are used to determine the evolution of the spall strength with sample temperature. They are complemented by post-test observations of the recovered targets, which reveal clear changes in fracture surface morphology in the spall craters. In the case of iron, possible influences of pressure-induced phase transformations prior to tensile loading are discussed on the basis of hydrodynamic simulations.
2:30PM V6.00004 Measurements of a Strength of Metals in a Picosecond Time Range, SERGEY ASHTIKOV, PAVEL KOMAROV, MIKHAIL AGRANAT, GENNADY KANEK, VLADIMIR FORTOV, Joint Institute for High Temperatures of Russian Academy of Sciences — We studied the shock-wave phenomena in metal films of a micron or submicron thickness irradiated by femtosecond laser pulses. The single-shot interferometer technique was used to record the time and spatial resolved displacements of both the frontal and rear surfaces of the films. The free surface displacement histories were converted into the free surface velocity histories using several various approaches. As a result, new data on the HEL and spall strength values have been obtained for aluminum, iron, nickel and other metals in strongly metastable states close to ultimate shear and tensile stresses. Comparison of measured parameters of elastic shock waves with the data of plate impact experiments at larger sample thicknesses demonstrate different regimes of the decay: whereas for pure fcc metals the decay may be described by one power function over 1 μm to 10 mm range of the distances, in the case of bcc iron main decay occurs obviously at the distance of order of 50 μm. The data are discussed from the view point of main mechanisms of high-rate deformation and fracture.

2:45PM V6.00005 Nanosecond to Picosecond Instability Regimes for Solids Under Large Deformation, R.A. GRAHAM, The Tome Group — Modeling of physical, chemical, and mechanical behaviors of solids under large finite deformation requires identification and measurement of often ambiguous, interacting behaviors. For times less than a few nanoseconds mechanical processes are not constrained by macroscopic conditions of uniaxial strain. Rather, behaviors are consequences of inertial responses controlled by crystallography, chemistry and morphology. At every moment - at each particular place - responses are born and Response may be inferred from related measurements as typically assumed. Nevertheless when combined with other excitations or unknown instabilities, originally unresolved events may be significant or dominant. Notable are: large magnetic fields, large electric fields, structured loading, instrumentation with piezoelectric crystals or optical windows, ferroelectric crystals or ceramics, polymers; as well as ballotistic reactions. Instabilities resulting from mass, thermal, thermochemical, or chemical accelerations (either, or, and) may readily lead to observable effects in interactive environments. Such instabilities are not quantitatively predictable today. Forward-looking modeling requires data from sub-nanosecond, three-dimensional acceleration measurements rather than engineering fixes. Interactions among mechanical, electronic, and optical processes are overt in the original piezoelectric 3-Zone Model of Neilson and Benedick [1], and recent and related work on finite-strain deformation science.


3:00PM V6.00006 XFEL diffraction of engineering materials under dynamic loading by nanoseconds laser pulse at SACLAC1, YUJI SANO, Toshiba, TOMOKAZU SANZ, NORIMASA OZAKI, Osaka Univ., TOSHIYUKI FUJITA, KEICHI HIROTA, SHIGEKIYA MIYASHITA, Toshiba, TOMOKI MATSUDA, HIROYUKI URANISHI, HYOYUKI KASHIWARA, YOSHIHIKO KONDO, TAKESHI MATSUOKA, Osaka Univ., KAZURO ARAKAWA, Shimane Univ., TAKAFUMI ADACHI, MAYU HASESHI, KIYOTAKA SATO, KANADE OGAWA, MAKANA YABASHI, RIHE, TADASHI OGASHI, KIYOKO TANAKA, KAZURO KODAMA, Osaka Univ. — Laser-induced plastic deformation imparts compressive residual stress and enhances the reliability of components. The authors studied the dynamic behavior of materials with XFEL during the plastic deformation. Foil of aluminum alloy was stuck on an acrylic plate with vacuum grease, through which a laser pulse of an Nd:YAG laser were irradiated. XFEL with energy of 10 kev impinged on the opposite free surface of the foil with various delay time and the diffraction was recorded with a two-dimensional detector (MPCCD). When the impulsive wave arrived at the opposite surface, the diffraction pattern obviously changed from spotty to a smoother ring pattern, suggesting the fragmentation of coarse grains. Shifts of diffraction angles were also observed.

1 The XFEL experiments were performed at the BL3 of SACLAC with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) (Proposal No. 2012A8012 and 2012B8011).

3:15PM V6.00007 Hopkinson pressure bar set-up for the measurement of Bauschinger effect under dynamic loading, ANDREW RUGGIERO, NICOLA BONORA, University of Cassino and Southern Lazio, GIANLUCA IANNITTI, Techdyn Engineering — Metals and alloys show different stress-strain characteristics under reverse loading cycle (Bauschinger effect). The knowledge of the effective material response is important in impact dynamics where material is subjected to compression-tension loading. In this paper an experimental set-up of the Hopkinson pressure bar to characterize the material response under dynamic loading cycle is presented. In the proposed configuration, in one single test, the sample is subjected to tension and compression loading with same absolute stress intensity and duration. Also this solution allows the possibility to select the load cycle sequence (tension-compression or compression-tension). Relationships to determine the stress, strain rate and strain from the elastic signals at the bars which are also effective for the second stress pulse, are presented. The method was verified with FEM and used to determine the Bauschinger effect for AISI 316L stainless steel.

3:30PM V6.00008 Modeling Single-Crystal Microstructure Evolution due to Shock Loading, JEFFREY LLOYD, Georgia Institute of Technology, JOHN CLAYTON, US Army Research Laboratory, DAVID MCDOWELL, Georgia Institute of Technology — An existing high strain rate viscoplastic (HSRVP) model is extended to address single-crystal anisotropic, elastic-plastic material response and is implemented into a steady plastic wave formulation in the weak shock regime. The single-crystal HSRVP model tracks nucleation, multiplication, annihilation, and trapping processes of dislocations, as well as thermal activated and phonon drag regimes. The steady plastic wave formulation is used to model the evolving elastic-plastic response with respect to a propagating longitudinal wave, and assumes that the magnitude of quasi-transverse waves is negligible. This steady wave analysis does not require specification of artificial viscosity, which can give rise to spurious dissipative effects. The constitutive model and its numerical implementation are applied to single-crystal pure Al and results are compared with existing experimental and computational data. Dislocation evolution, lattice reorientation, and macroscopic velocity-time histories are tracked for different initial orientations subjected to varying peak shock pressures. Results suggest that initial material orientation can significantly influence microstructure evolution, which in turn has been shown to influence damage behavior during tensile unloading.

Thursday, July 11, 2013 1:45PM - 3:30PM –
Session V7 CH.2 Chemistry: Optical Initiation
Grand Crescent - Brian Jensen, Los Alamos National Laboratory

1:45PM V7.00001 Nonlinear optical techniques and optical properties of condensed molecular systems, MARGHERITA CITRONI, LENS - European Laboratory for Non Linear Spectroscopy, University of Florence — Structure, dynamics, and optical properties of molecular systems can be largely modified by the applied pressure, with remarkable consequences on their chemical stability. Several examples of selective reactions yielding technologically attractive products can be cited, which are particularly efficient when photochemical effects are exploited in conjunction with the structural conditions attained at high density. Non-linear optical techniques are a basic tool to unveil key aspects of the chemical reactivity and dynamic properties of molecules. Their application to high-pressure samples is experimentally challenging, mainly because of the small sample dimensions and of the non-linear effects generated in the anvil materials. In this talk I will present results on the electronic spectra of several aromatic crystals obtained through two-photon induced fluorescence and two-photon excitation profiles measured as a function of pressure (typically up to about 25 GPa), and discuss the relationship between the pressure-induced modifications of the electronic structure and the chemical reactivity at high pressure. I will also present the first successful pump-probe infrared measurement performed as a function of pressure on a condensed molecular system. The system under examination is liquid water, in a sapphire anvil cell, up to 1 GPa along isotherms at 298 and 363 K. These measurements give a new enlightening insight into the dynamical properties of low- and high-density water allowing a definition of the two structures.
2:15PM V7.00002 High pressure chemistry of red phosphorous by photoactivated simple molecules, MATTEO CEPPATI, ICCOM-CNRS and LENS, ROBERTO BINI, SAMUELE FANELTI, LENS and University of Florence, MARIA CAPORALI, MAURIZIO PERUZZINI, ICCOM-CNRS — High pressure (HP) is very effective in reducing intermolecular distances and inducing unexpected chemical reactions. In particular the photoactivation of the reactants in HP conditions can lead to very efficient and selective processes. The chemistry of phosphorous is currently based on the reactive form. The red polymeric allotrope, despite more stable and much less toxic, has not attracted much attention so far. However, switching from the red form would benefit any industrial procedure, especially from an environmental point of view. On the other side, water and ethanol are renewable, environmentally friendly and largely available molecules, usable as reactants and photoactivators in HP conditions. Here we report a study on the HP induced reactivity of red phosphorous with water and ethanol, showing the possibility of very efficient and selective processes, leading to molecular hydrogen and valuable phosphorus compounds. The reactions have been studied by means of FTIR and Raman spectroscopy and pressure has been generated using DAC and SAC. HP reactivity has been activated by the two-photon absorption of near-UV wavelengths and occurred in total absence of solvents, catalysts and radical initiators, at room T and mild pressure conditions (0.2-1.5 GPa).

2:30PM V7.00003 Studies in useful hard x-ray induced chemistry, MICHAEL PRAVICA, LIGANG BAI, DANIEL SNEED, University of Nevada, Las Vegas, CHANGYONG PARK, HP-CAT, Carnegie Geophysical Laboratory — The observed rapid decomposition of potassium chloride (via 2KClO3 + hν → 2KCl + 3O2) via synchrotron hard x-ray irradiation (>10 keV) has enabled experiments that are developing novel and useful hard x-ray chemistry. We have observed a number of radiation-induced in situ decomposition reactions in various substances which release O2, H2, N2, NH3, and H2O in a diamond anvil cell (DAC) at ambient and high pressures. These novel acalycytic and isothermal reactions are seen as a highly controllable, penetrating, and focused method to initiate chemistry (including x-ray induced combustion) in sealed and/or isolated chambers which maintain matter under extreme conditions. During our studies, we have typically observed a slowing of decomposition with pressure including phase dependent decomposition of KClO3. Energy dependent studies have observed an apparent resonance near 15 keV at which the decomposition rate is maximized. This may enable use of much lower flux and portable x-ray sources (e.g., x-ray tubes) in larger scale experiments. These developments support novel means to load DACs and control chemical reactions providing novel routes of synthesis of novel materials under extreme conditions.

2:45PM V7.00004 Structural characterization of high-pressure liquid water by transient infrared ultrafast spectroscopy, SAMUELE FANELTI, LENS, European Laboratory for Non-linear Spectroscopy, ANDREA LAPINI, MARCO PAGLIAI, MARGHERITA CITRINO, MARIANGELA DI DONATO, LENS and “Ugo Schiff” Chemistry department, University of Florence — Experimental and computational studies have reported in the last years the existence of two different local structures of liquid water depending on pressure and temperature conditions, called low density (LDW) and high density (HDW). For the first time we have combined pump-probe ultrafast spectroscopy with ultra high pressure devices to access the gigapascal range, providing new insights on the understanding of the two structures peculiarities and their interconversion, in the whole range of thermodynamic stability of liquid water, from 273 to 363 K from ambient pressure up to 1.2 GPa. We measured the OD stretching rotational anisotropy decay time-constant and vibrational lifetime T1, in a solution of HOD in H2O, pressurized in a sapphire anvil cell, as a function of pressure at different temperatures and we performed a careful infrared linewidth study of the OD stretching mode as a function of temperature and pressure. We interpreted the pressure evolution of the measured parameters in terms of structural changes, identifying the key to correlate the structure evolution with the dynamic data that led us to define the pressure and temperature region where only HDW exists.

3:00PM V7.00005 Transient Absorption and Hugoniot Equations of State of Shocked Reactive Liquids, KATHRYN BROWN, SHAWN MCGHRANE, PETER SCHULZIE, NHAN DANG, DAVID MOORE, Los Alamos National Laboratory — We use transient absorption spectroscopy and ultrafast dynamic ellipsometry (UDE) to characterize reactions that occur in reactive liquid thin layers, including nitromethane and carbon disulfide, that have been subjected to sustained (~300 ps) shocks up to <20 GPa from an amplified Ti:sapphire laser. Shock compression can cause some liquids to react and form new chemical species. Though not chemical-specific, transient absorption and deviations from the universal liquid Hugoniot can indicate the presence of chemical reactions taking place. The information obtained from these experiments can be applied to more specific characterization methods such as vibrational spectroscopy.

3:15PM V7.00006 Transformation of Simple Molecular Fluids to Conducting States in the Laser-Heated Diamond Anvil Cell, R.S. MCVILLIAMS, Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C. 20015, D.A. DALTON, Defense Threat Reduction Agency, Fort Belvoir, V.A., 22060, M.F. MAHMOOD, Howard University, Washington D.C., 20059, A.F. GONCHAROV, Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C., 20005 — The nature of high-pressure, high-temperature chemical and electronic transformation of simple molecular and small molecules such as hydrogen and nitrogen is a subject of ongoing study and many open questions. Particularly challenging is the laboratory study of states corresponding with fluid-fluid phase transformations, from insulator to conductor and/or molecular to non-molecular. These may take the form of first-order (i.e. discontinuous in P and T) phase boundaries at conditions yet to be explored completely by experiments. Previously, such states were accessible solely via dynamic compression techniques, however limitations in experimental geometry and timescale and confinement to adiabatic pathways has limited the range of conditions accessed and the variety of measurements available. New developments in static compression, involving the acceleration of laser-heated diamond-anvil-cell experiments to microsecond timescales via fast spectroscopy, enable study of this interesting regime in hydrogen and nitrogen as well as novel measurements of material state. These results complement dynamic compression data and extend measurements to previously unexplored conditions where first-order liquid-liquid transformations have been predicted.
4:15PM W1.00002 X-ray microtomography study of the spallation response in Ta-W , SAMUEL MCDONALD, School of Materials, University of Manchester, Manchester, M13 9PL, United Kingdom, MATTHEW COTTON, JEREMY MILLETT, NEIL BOURNE, AWE, Aldermaston, Reading, Berkshire, RG7 4PR, United Kingdom, PHILIP WITHERS, School of Materials, University of Manchester, Manchester, M13 9PL, United Kingdom — The response of metallic materials to high strain-rate (impact) loading is of interest to a number of communities. Traditionally, the largest driver has been the military, in its need to understand armour and resistance to ballistic attack. More recently, industries such as aerospace (foreign object damage, bird strike, etc.), automotive (crash-worthiness) and satellite protection (orbital debris) have all appreciated the necessity of such information. It is therefore important to understand the dynamic response of materials to spallation loading, and in particular to be able to observe in three-dimensions, and in a non-invasive manner, how the physical damage present in the spalled region post-impact. The current study presents plate impact experiments investigating the spallation damage response of recovered targets of the tantalum alloy Ta-2.5%W. Using X-ray microtomography the damage resulting from differing impact conditions (impact velocity/stress, pulse duration) is compared and characterised in 3-D. Combined with free surface velocity measurements, the tensile failure mechanisms during dynamic loading have been identified.

4:30PM W1.00003 Effect of Pre-Strain on the Twinning Behavior in Tantalum , JEFFREY FLORANDO, NATHAN BARTON, BASSEM EL-DASHER, MUKUL KUMAR, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, CHANGQIANG CHEN, Northwestern University, KALIAT RAMESH, KEVIN HEMKER, Johns Hopkins University — In an effort to understand the relationship between the mobile dislocation density and twinning, polycrystalline Ta samples have been pre-strained to various amounts of strain at room temperature, and then tested at liquid nitrogen temperatures at a strain rate of 1/s, and under laser-induced shock wave loading; conditions that promote twinning. Recovered samples were characterized using EBSD orientation mapping along with transmission electron microscopy to assess the occurrence of twinning under each test condition. The results show that as the dislocation density increases, there are discernible differences in the initial portion of the stress-strain and wave profile data which can be linked to the amount of twinning observed. In addition, the experimental observations have been compared with a crystal level twinning model. The implications of these findings on the deformation behavior will be discussed.

4:45PM W1.00004 The Influence of Shock-Loading Path on the Spallation Response of Ta , GEORGE GRAY III, Los Alamos National Laboratory, Los Alamos, NM 87545, NEIL BOURNE, AWE Aldermaston, Reading, Berkshire, RG7 4PR, UK, VERONICA LIVESCU, CARL TRUJILLO, Los Alamos National Laboratory, Los Alamos, NM 87545, SAM MCDONALD, University of Manchester, Sackville Street, Manchester, M60 1QR, UK, DYNAMIC PROPERTIES TEAM COLLABORATION, AWE COLLABORATION, MANCHESTER UNIVERSITY COLLABORATION — Spallation is well known to be a complex process strongly influenced by microstructure, loading path, and the loading profile yet often a singular “spall strength” is utilized in hydrocodes to quantify the dynamic fracture behavior of a material. In this study the influence of loading path on the “spall strength” and damage evolution in high-purity Ta is presented. The Ta samples where shock loaded to three peak shock stresses using both symmetric impact and two different composite flyer plate configurations such that upon unloading the three samples displayed nearly identical “pull-bac” signals as measured via rear-surface velocimetry. While the “pull-bac” signals are very similar in magnitude, the highest peak stressed sample resulted in complete spall scab separation while the two lower peak stresses resulted in incipient spall. The damage evolution in the “soft” recovered Ta samples was quantified using optical metallography, electron-back-scatter diffraction, and tomography. The effect of loading path on spallation and its ramifications for the stress and kinetic dependency of dynamic damage evolution is discussed.

5:00PM W1.00005 Plastic flow, inferred strength, and incipient failure in BCC metals at high pressures, strains, and strain rates , HYE-SOOK PARK, LLNL — We present our extensive experimental results from the Omega laser to test models of high pressure, high strain rate strength at ~ 1 Mbar peak pressures, strains >10%, and strain rates of ~ 10^7 s^-1 in Ta, V, and Fe, using plastic flows driven by the Rayleigh-Taylor instability. The observed time evolution of the plastic deformation is compared with 2D simulations incorporating a strength model. This methodology allows average values of strength at peak pressure and peak strain rate conditions to be inferred. The observed values of strength are typically factors of 5-10 higher than ambient strength, with contributions coming from pressure hardening (via the shear modulus), and strain rate hardening. For Fe, there is the added contribution from the alpha-epsilon phase transition. Ta has been studied as a function of grain size, and at the high strain rates and short durations of the experiments, no grain size dependence was observed; the observed deformation and inferred strength were independent of grain size. Both Ta and V have been driven to large enough strains that incipient failure (softening) has been observed. Both the Ta and V experiments were compared favorably with multiscale strength models, with the conclusion that the Ta deformation was in the thermal activation regime, whereas the V deformation was in the phonon drag regime. Finally, preliminary results of new iron RT strength experiments done at ~ 1 Mbar pressures, and ~ 10^7 s^-1 strain rates, well beyond the alpha-epsilon phase transition, will be given.

5:30PM W1.00006 ABSTRACT WITHDRAWN —

5:45PM W1.00007 Study of Materials at High Negative Pressures Using Picosecond Laser Pulses , I.K. KRASYUK, S.A. ABROSIMOV, A.P. BAZHULIN, P.P. PASHININ, A. YU. SEMENOV, I.A. STUChEBRYUKHOV, V.V. VORONOv, C.P. RAS, Moscow, Russia, K.V. KHISHChENko, JIHT RAS, Moscow, Russia — In the present work, the dynamic strength of Al, Pb, Cu, and Ta was studied by the method of generation of shock waves under the action of laser pulses of 70 ps duration. The use of such short pulse make it possible to realize in the experiments strain rates exceeding 10^7 s^-1. We have used an approach that is based on both the measurement of the spallation depth after the pulse-action on the target and the subsequent numerical simulation of the shock-wave process in the matter under study. The obtained data show that, at moderate amplitudes of shock loading, spall strength values are in a good agreement with the known functional dependencies of the strength upon the rate of deformation. With greater loading pressure, a sharp growth of spall strength, that indicates the strengthening of the material as a result of loading, takes place. The registered growth of spall strength of the metals is connected with the fact that, in the experiments, the increase of the rate of deformation was achieved not only by shortening of the pulse duration, but also by the increase of the amplitude of loading. The latter increase leads to hardening of the material under study. In this case, defects, which cause the premature spallation of the material, may be disappeared.

Thursday, July 11, 2013 4:00PM - 6:00PM
Session W2 HM High Energy Density Materials II
Elliott Bay - Michael Desjarlais, Sandia National Laboratories

4:00PM W2.00001 Inertial Confinement Fusion as an Extreme Example of Dynamic Compression , E. MOSES , Lawrence Livermore National Laboratory — Initiating and controlling thermonuclear burn at the national ignition facility (NIF) will require the manipulation of matter to extreme energy densities. We will discuss recent advances in both controlling the dynamic compression of ignition targets and our understanding of the physical states and processes leading to ignition.
High-pressure studies on fundamental physics and chemistry, especially on the Earth and planetary sciences, have been enormous. While experiments in diamond anvil cells (DACs) at pressures of ~250 - 400 GPa are proven to be very difficult but possible, at higher static pressures any matter has not been investigated so until very recently [Ref. 1]. We have developed a method of synthesis of balls and semi-balls (of 10 to 50 µm in diameter) made of nanodiamond (with individual nano-particles of linear dimensions below 100 nm) and used them as second-stage or indentor-type anvils in conventional DACs. In experiments on rhenium, osmium, and gold we were able to generate pressures above 650 GPa [Ref. 1] and demonstrated crucial necessity of the ultra-high pressure measurements for accurate determination of the equation of state (EOS) of materials at extreme conditions.

In collaboration with Leonid Dubrovinsky, Bayerisches Geoinstitut, University of Bayreuth; Vitali Prakapenka, University of Chicago; Artem Abukumov, University of Antwerp, and Michael Hanfland, ESRF, Grenoble.


5:00PM W2.00003 Isochoric heating using proton beams and shock compression generated by UHF lasers , MARKUS ROTH, Technische Universität Darmstadt — Material conditions in the Warm Dense Matter (WDM) regime are of great interest for high energy density physics, the development of controlled thermonuclear fusion and astrophysics. Each experiment involving high energy deposition will be strongly affected by the sample’s changed behavior in the WDM regime. In particular, carbon is an interesting material for warm dense matter studies, as it is accessible experimentally since carbon samples can easily be manufactured and handled in the laboratory. Due to its low number of electrons, a number of theoretical and numerical techniques, including ab-initio simulations, allow for the description of its properties within the computational resources available today. Additionally, the solid-liquid phase transition of carbon is in the warm dense matter regime and may play a major role in the physics of ice giants like Neptune and Uranus [1, 2] and white dwarfs [3]. This transition is poorly understood so far and further investigation is needed [4]. In fact, the solid-liquid phase transition on the graphite Hugoniot has never been measured reliably so far. A recent new option is the use of x-rays which are able to access the processes inside the sample. In comparison to radiography x-ray scattering cannot only measure the propagation of a shock but also the microscopic structure inside the sample [5, 6, 7]. Thus, strong changes in the structure due to the phase transitions induced by shock or isochoric heating can be measured directly. The creation of fluid carbon requires a rapid energy input, preferably into a large volume. Ion beams are a unique tool for that task as they deposit their energy deep in the sample [5, 6, 7]. Thus, strong changes in the structure due to the phase transitions induced by shock or isochoric heating can be measured directly. This method was first applied for the carbon solid-liquid phase transition at lower pressure in a proof-of-principle experiment where the isochoric heating was realized by laser-accelerated protons [8]. However, in this first experiment only the relative increase of the total scattering signal was measured. It was not possible to distinguish between the elastic and inelastic features. In the experiment presented in this talk, we have obtained frequency-resolved scattering spectra, which allow to study the evolution of both the elastic and the inelastic features separately.


5:30PM W2.00004 Astrophysical experiments at a gigabar on the National Ignition Facilityi , A. KRITCHER, D.C. SWIFT, T. DOEPPNER, J.A. HAVRELIAK, J. EGGERT, G.W. COLLINS, S. GLENZER, Lawrence Livermore National Laboratory, R. FALCONE, University of California - Berkeley, P. NEUMAYER, GSI Darmstadt — We have now demonstrated a capability at NIF to produce accurate equation of state (EOS) measurements on matter into the gigabar regime. Work so far has focused on CH, but with further development it will be possible to study other materials, in particular of higher Z. As well as being relevant to high-pressure engineering systems such as inertial confinement fusion, we can address key problems in astrophysics. Gigabar-scale pressures occur within massive exoplanets, and experimentally-constrained EOS measurements are essential to interpret exoplanet observations in terms of internal structures. This research provides important constraints for assessments of dark matter, by improving estimates of the total amount of baryonic mass for a given density of luminous (stellar) mass, because the ratio of non-luminous to luminous mass depends on the upper mass limit of brown dwarfs, which depends sensitively on the EOS. We are also able in NIF experiments to deduce the opacity along the shock Hugoniot, which is a necessary component in studies of stellar structure and evolution.

iThis work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

5:45PM W2.00005 Thermodynamic and transport properties along Jupiter’s adiabat , MARTIN FRENCH, Sandia National Laboratories, ANDREAS BECKER, WINFRIED LORENZEN, University of Rostock, NADINE NETTELMANN, University of California, Santa Cruz, MANDY BETHKENHAGEN, University of Rostock, JOHANNES WICHT, Max Planck Institute for Solar System Research, Katlenburg-Lindau, THOMAS MATTSSON, Sandia National Laboratories, RONALD REDMER, University of Rostock — Accurate knowledge about the behavior of the major constituents, hydrogen and helium, is required to model and understand the interior of Jupiter. Transport properties like the thermal and electrical conductivity as well as the viscosity are particularly interesting to examine, since their behavior changes drastically at the transition from the dense nonideal plasma to the molecular fluid. Here we use ab initio molecular dynamics simulations based on density functional theory to calculate equilibrium and transport properties of the warm dense H-He mixture. In particular, we present results [1] for thermodynamic material properties, the shear and longitudinal viscosity, the electrical and the thermal conductivity in hydrogen-helium mixtures along the isentrope of Jupiter. Our results cover the range from the outer molecular regions (2000 K, 5 kbar) to the core-mantle boundary (19000 K, 40 Mbar). These new data will lead, e.g., to significant improvements in understanding the origin and shape of the magnetic field of Jupiter.

Bragg grating sensors have predictable thermal and mechanical response properties with pressure spectrally shifting the reflectance peak at an embedded probe (single-mode 1550 nm fiber-based Bragg grating - FBG) that provides a continuous fast pressure record during shock and/or detonation. Fiber grating sensors to obtain high temporal resolution in situ pressure measurements in inert materials under precise shock loading from a gas-gun driven to-detonation tests (DDT), where pressure and temperature were measured to 82 kbar and 400 °C temperature measurements under dynamic conditions by using an all-optical fiber-based approach. While similar tests have been done previously in deflagration-DATTELBAUM, Los Alamos National Laboratory, ERIC UDD, Columbia Gorge Research — We present a new technique for simultaneous, in situ pressure and temperature of energetic materials during the early stages of detonation and the transition to full detonation represents a significant advance in diagnostic capabilities. These measurements provide insight into this dynamic regime detonation physics. Continuous velocity and burn back position measurements are significantly more accurate in determining this run-up in velocity relative to single point measurements which yield only the average velocity measurement. These measurements during burn, deflagration and detonation of energetic materials including explosives and rocket propellant in Russian DDT tests. For the first time explosive. However, the dielectric constant of HMX-based explosives has been measured only over a small range of wavelengths. Here we employ an open-ended coaxial probe to determine the complex dielectric constant for LX-10 and other HMX-based explosives over the full 5-50 GHz range. The development and propagation of detonation waves in both heavy- and lightly-confined cylindrical charge geometries will also be highlighted. In some experiments the microwave reflective properties of the region behind the detonation front are characterized by using a remotely-positioned microwave waveguide probe. Ionization pins and Manganin gauges were used with microwaves simultaneously to verify the technique as the detonation front progresses.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Microwave interferometry is a useful technique for understanding the development and propagation of detonation waves. The velocity of the front can be determined directly with the instantaneous phase difference of the reflected microwave signal from the detonation front and the dielectric constant of the explosive. However, the dielectric constant of HMX-based explosives has been measured only over a small range of wavelengths. Here we employ an open-ended coaxial probe to determine the complex dielectric constant for LX-10 and other HMX-based explosives over the full 5-50 GHz range. The development and propagation of detonation waves in both heavy- and lightly-confined cylindrical charge geometries will also be highlighted. In some experiments the microwave reflective properties of the region behind the detonation front are characterized by using a remotely-positioned microwave waveguide probe. Ionization pins and Manganin gauges were used with microwaves simultaneously to verify the technique as the detonation front progresses.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Dielectric characterization and microwave interferometry of HMX-based explosives1, JOSEPH TRINGE, RON KANE, THOMAS LORENZ, EMER BALUYOT, KEVIN VANDERSALL, Lawrence Livermore National Laboratory — Microwave interferometry is a useful technique for understanding the development and propagation of detonation waves. The velocity of the front can be determined directly with the instantaneous phase difference of the reflected microwave signal from the detonation front and the dielectric constant of the explosive. However, the dielectric constant of HMX-based explosives has been measured only over a small range of wavelengths. Here we employ an open-ended coaxial probe to determine the complex dielectric constant for LX-10 and other HMX-based explosives over the full 5-50 GHz range. The development and propagation of detonation waves in both heavy- and lightly-confined cylindrical charge geometries will also be highlighted. In some experiments the microwave reflective properties of the region behind the detonation front are characterized by using a remotely-positioned microwave waveguide probe. Ionization pins and Manganin gauges were used with microwaves simultaneously to verify the technique as the detonation front progresses.

1 This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Rubidium Atomic Line Filtered (RALF) Doppler Velocimetry. MARIO FAJARDO, CHRISTOPHER MOLEK, ANNAMARIA VESELY, US Air Force Research Lab, LASEM TEAM — We report our progress towards adapting the well-known Global Dopper Velocimetry (GDV) technique, popular in the aerodynamics community, to the order-of-magnitude higher velocities pertinent to shock experiments. In GDV, the narrow-line illumination laser is tuned to an edge of a molecular iodine absorption line; an iodine gas cell converts the Doppler shift of the reflected light to transmitted intensity. We follow the suggestion in the original 1990 patent by Komine and broaden the absorption lines of alkali metal atoms by adding a buffer gas, thereby tuning the transmission edge spectrum to match the Doppler shift (surface velocity) range of interest. We use atomic rubidium vapor cells, with 0 to 1 atmosphere pressures of molecular nitrogen buffer gas, and coin the name “Rubidium Atomic Line Filtered” (RALF) Doppler velocimetry. [96ABW-2013-0036]

Fiber Bragg Grating sensor for shock wave diagnostics. AVI RAVID, EHUD SHAFIR, SHLOMI ZILBERMAN, GARRY BERKOVIC, BENNY GLAM, GABRIEL APPELBAUM, Applied Physics Division, Soreq NRC, 51800 Yavne, Israel — Fiber Bragg Grating (FBG) sensor response was studied in gas-gun shock wave experiments. The sensors were embedded in PMMA target subjected to planar shock waves under IGP. Two orientations of the FBG sensor with respect to the shock plane were examined: parallel and perpendicular. The shift of the reflected wavelength was measured with a system based on commonly available communication grade add-drop filters that covered the maximal expected wavelength swing. The FBG sensors survived the shock and their strain-to-wavelength response was determined by comparison to the calculated strain based on the known PMMA EOS and VISAR measurements.

Fiber Grating Sensor System to Measure Velocity, Position, Pressure, and Temperature during Burn, Deflagration and Detonation of Highly Energetic Materials. ERIC UDD, Columbia Gorge Research, LLC — A novel very high speed fiber grating sensor system has been used to support velocity, position, temperature and pressure measurements during burn, deflagration and detonation of energetic materials including explosives and rocket propellant in Russian DDT tests. For the first time the system has been demonstrated in card gap testing and has allowed real time measurements of the position of the blast front into the card gap and monitoring of pressure at key locations in the card gap test. Fiber grating sensors are capable of providing a continuous measurement of the position, velocity, local pressure and temperature of energetic materials during the early stages of detonation and the transition to full detonation represents a significant advance in diagnostic capabilities. These measurements provide insight into this dynamic regime detonation physics. Continuous velocity and burn back position measurements are significantly more accurate in determining this run-up in velocity relative to single point measurements which yield only the average velocity measurement between the individual pin placement points. This work describes the first demonstration of this technology to card gap testing.

Embedded optical probes for simultaneous pressure and temperature measurement of materials in extreme conditions. RICHARD L. SANDBERG, GEORGE RODRIGUEZ, LEE GIBSON, DANA M. DATTELBAUM, Los Alamos National Laboratory, ERIC UDD, Columbia Gorge Research — We present a new technique for simultaneous, in situ pressure and temperature measurements under dynamic conditions by using an all-optical fiber-based approach. While similar tests have been done previously in deflagration-to-detonation tests (DDT), where pressure and temperature were measured to 62 kbar and 400 °C simultaneously, here we demonstrate the use of embedded fiber grating sensors to obtain high temporal resolution in situ pressure measurements in inert materials under precise shock loading from a gas-gun driven plate impact. The system capitalizes on existing telecom components and fast transient digitizing recording technology. It operates as a relatively inexpensive embedded probe (single-mode 1550 nm fiber-based Bragg grating - FBG) that provides a continuous fast pressure record during shock and/or detonation. Fiber Bragg grating sensors have predictable thermal and mechanical response properties with pressure spectrally shifting the reflectance peak at λ =1550 nm to the blue and temperature shifting the peak to the red. By applying well-controlled steady shock wave pressure profiles to soft materials such as PMMA, we study the dynamic pressure response of embedded fiber Bragg grating to extract pressure amplitude of the shock wave and compare our results with in situ particle velocity wave profiles measured simultaneously.
interface characteristics that cause these two types of interfaces to nucleate and transmit dislocations by significantly different mechanisms. Critical shock pressures to nucleate from and are lower than 10 nm, controlling their plasticity. The preferred nucleation sites are found to be closely associated with the interface misfit dislocation structures, shock compression. We found that Shockley partials prefer to nucleate from the interface and then transmit into the neighboring layers when the layer thicknesses orientation relationship, to provide insight into the role of interface structure on the nucleation, transmission, absorption, and storage of dislocations during.

The Cu-Nb system, large-scale molecular dynamics simulations are performed on two interfaces, Kurdjumov-Sachs, RUIFENG ZHANG, T.C. GERMANN, I.J. BEYERLEIN, X.Y. LIU, JIAN WANG, Los Alamos National Lab — Using newly constructed interatomic potential SeCTyP U. N. Cuyo and PICT2008-1325.

1Supported by the Department of Energy for Los Alamos National Security LLC under Contract no. DE-AC52-06NA25396.

Thursday, July 11, 2013 4:00PM - 6:00PM – Session W4 TM Molecular Dynamics IV Vashon - Sandro Scandolo, International Centre for Theoretical Physics

4:00PM W4.00001 Unrevealing transition mechanism: novel carbons, metallic germaniums, and low-temperature galliums, DANIELE SELL, IGOR A. BABURIN, Technische Universität Dresden, ROMAN MARTONÁK, Comenius University, STEFANO LEONI, Technische Universität Dresden — The quest for novel carbon-based materials is a topic of high priority. Using accelerated molecular dynamics techniques we investigated low-temperature compression of graphite into novel carbon modifications with odd-even topological pattern. At room temperature germanium modifications shows semiconducting properties, while metallicity and superconductivity have been found, so far, only in high pressure modifications. By means of different theoretical methodology, we are able to predict new semiconducting and low pressure metallic Ge phases together with a clearer picture of particular transformation paths and specific indication of possible synthesizabilities. Gallium is among the most challenging elements of the periodic systems. Its polymorphs are structurally very peculiar, characterized by unusual open ground-state crystal structures. While high-pressure promotes close-packed galliums, low-temperature, and the use of mild oxidative chemical approaches, is a way of affecting nucleation patterns towards novel open, clathrate-like compounds.

4:15PM W4.00002 Frictional Interactions at High Velocity Polycrystalline Ductile Metal Interfaces1, JAMES HAMMERBERG, JACQUELINE MILHANS, RAMEO RAVOLO, TIMOTHY GERMANN, Los Alamos National Laboratory — We have examined the effect of evolution of grain morphology on the frictional force at polycrystalline Al-Al and Al-Ta interfaces as a function of grain size and sliding velocity. We present the results of 8M, 26M and 138M particle NonEquilibrium Molecular Dynamics (NEMD) simulations for grain sizes of 13.5, 19.3 and 20 nm. Sample sizes consisted of 3x3x3 and 5x5x5 grains on each side of a sliding interface. We have considered sliding velocities of 42, 50, 100, 140, and 240 m/s. For velocities below a size dependent critical velocity above which a fluid layer forms, we find enhanced grain coarsening leading to a highly strained, graded final steady state microstructure that exhibits a dynamic morphology for times greater than 5-10 ns. We find that the frictional force is insensitive to the initial grain size distribution due to the evolution of the initial distribution to a new nonequilibrium steady state. We discuss the relationship of these results to single crystal interfaces and the mechanisms for grain size and shape evolution.

1This work supported by the U.S. Department of Energy under contract DE-AC52-06NA25396.

4:30PM W4.00003 Large-scale Molecular Dynamics Simulations of Shock-induced Plasticity and Twinning in bcc Nb and Ta, TIMOTHY GERMANN, RUIFENG ZHANG, Los Alamos National Laboratory, RAMON RAVOLO, University of Texas at El Paso — Large-scale classical molecular dynamics (MD) simulations are used to investigate dislocation slip and twinning activity in bcc metals under shock compression. We will discuss both the orientation-dependent response of Nb and Ta single crystals, as well as the more complex response of nanocrystalline samples. Of particular importance as MD simulations are becoming applied to model more complex materials, we will discuss issues related to the interatomic potential description and the analysis of the deformation response. Embedded atom method (EAM) potentials for shock compression studies must properly describe the energy landscape under the pressure range of interest; and an orientation imaging map technique is described for following the plastic response of fcc and bcc metals.

4:45PM W4.00004 Shock waves in polycrystalline iron: plasticity and phase transitions1, EDUARDO BRINGA, CONICEIT and Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, Argentina, NINA GUNKELMANN, Physics Department and Research Center OPTIMAS, University Kaiserslautern, Kaiserslautern, Germany, CARLOS RUESTES, Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, Argentina, HERBERT URBASSEK, Physics Department and Research Center OPTIMAS, University Kaiserslautern, Kaiserslautern, Germany — Iron undergoes a bcc to close-packed structural phase transition under pressure, at around 13 GPa. Atomicistic simulations have been able to provide insights into the transition, but without dislocation plasticity occurring before the phase change, while experiments in polycrystals do show clear evidence for dislocation plasticity. Here we study shock waves in polycrystalline Fe using two different interatomic potentials, below and above the phase transition pressure. We show that it is essential to employ a finite ramp time of the shock wave in the crystal in order to give dislocations sufficient time for nucleation. For grain sizes below 10 nm, where a significant fraction of the plastic activity can occur by grain boundary sliding, dislocation nucleation still is a relatively small contribution to shear stress relaxation.

1NG and HMU thank support from the Deutsche Forschungsgemeinschaft via the Sonderforschungsbereich 926. CJR and EMB thank support from ScCTyP U. N. Cuyo and PICT2008-1325.

5:00PM W4.00005 Role of Shock Response of Cu-Nb Nanolaminated Composites, RUIFENG ZHANG, T.C. GERMANN, I.J. BEYERLEIN, X.Y. LIU, JIAN WANG, Los Alamos National Lab — Using newly constructed interatomic potential for Cu-Nb system, large-scale molecular dynamics simulations are performed on two interfaces, Kurdjumov-Sachs {111}Cu/{110}Nb (KS) and {112}KS orientation relationship, to provide insight into the role of interface structure on the nucleation, transmission, absorption, and storage of dislocations during shock compression. We found that Shockley partials prefer to nucleate from the interface and then transmit into the neighboring layers when the layer thicknesses are lower than 10 nm, controlling their plasticity. The preferred nucleation sites are found to be closely associated with the interface misfit dislocation structures, and dislocation transmission abides by the geometrical compatibility of pairs of slip systems of adjoining crystals. Critical shock pressures to nucleate from and transmit dislocations across the atomically flat interface are shown to be substantially higher than those for the faceted interface. We discuss the atomic-level interface characteristics that cause these two types of interfaces to nucleate and transmit dislocations by significantly different mechanisms.
5:15PM W4.00006 Plasticity mechanisms in nanovoided b.c.c. metals under high strain rate compression¹, CARLOS J. RUESTES, Instituto de Ciencias Basicas, UNCuyo, Mendoza 5500, Argentina, EDUARDO M. BRINGA, Instituto de Ciencias Basicas & CONICET, UNCuyo, Mendoza 5500, Argentina, ALEXANDER STUKOWSKI, Technische Universitat Darmstadt, Germany, JOAQUIN F. RODRÍGUEZ NIEVA, Massachusetts Institute of Technology, MA 02139, USA, GRACIELA BERTOLINO, CONICET - Centro Atomico Bariloche, Bariloche 8400, Argentina, YIZHE TANG, Johns Hopkins University, Baltimore, MD 21212, USA, MARC A. MEYERS, University of California, San Diego, La Jolla, CA 92093, USA — Atomic-scale simulations provide unique insights to plasticity mechanisms arising under extreme conditions where its relative nanoscopic length and time scales render experiments almost impossible. Our studies explore the mechanical response and plasticity effects under uniaxial high strain rate compression for a Ta single crystal with a collection of spherical nanovoids, with a radius of 3-4 nm, providing an initial porosity of 5%-20%. We examine strain rate effects, from $10^7$/s to $10^{10}$/s, in the dislocation density and dislocation-induced heating. The resulting dislocation densities are in good agreement with experimental results for shock-recovered samples.

5:30PM W4.00007 MD-generated molecular volumes and their mechanical applications, NOHAM WEINBERG, University of the Fraser Valley, Simon Fraser University — Experimentally, the effects of pressure on reaction rates are described by their pressure derivatives, known as volumes of activation. Transition state theory directly links activation volumes to partial molar volumes of reactant and transition states. Traditionally, the experimentally measured effects of pressure on reaction rates are expressed in terms of so-called volumes of activation, which represent the difference in volumes of transition states and reactants. Since the volumes of reactants are readily available experimentally, the volumes of activation provide a direct measure of the transition state volumes. In this context, a reliable technique is required for relating the volume of a microscopic system to its geometrical parameters. Until recently, such a technique did not exist. Over the past five years we developed a precise method based on molecular dynamics simulations and applied it to calculation of molecular volumes and volumes of activation. The results of calculations closely matched the experimental values. We are now extending and refining this method in its application to a wider range of reactions, including biochemical processes and processes at extreme pressures.

5:45PM W4.00008 Equation of state and stability of metal crystals at high pressure by DFT calculations¹, DMITRY MINAKOV, PAVEL LEVASHOV, Joint Institute for High Temperatures of the Russian Academy of Sciences — In this work we present ab initio equation-of-state calculations for crystals of some metals. Density functional theory at finite temperature (VASP code) is used to obtain the properties of electrons; lattice is simulated in quasi-harmonic approximation at non-zero temperature of electrons. Anharmonic effects are taken into account by the thermal expansion of a crystal. All calculations were performed for aluminum, copper and gold. We compare our results with available shock-wave data in crystal phase, including isentropic expansion. The melting curves are calculated by different criteria; the effect of different temperatures of electrons and ions is taken into account. Also we determine thermodynamic and kinetic boundaries of stability of crystals. Our calculations demonstrate that ab initio approaches can be used to theoretically reconstruct thermodynamically complete EOS of metallic crystals.

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This work was supported by RFBR grant 12-08-31475 mol a.

Thursday, August 15, 2013 4:00PM - 6:00PM — Session W5 GP2: Planetary I. Cascade I - Alex Goncharov, Carnegie Institution for Science

4:00PM W5.00001 Probing planetary interiors: Shock compression of water to 700 GPa and 3.8 g/cc, and recent high precision Hugoniot measurements of deuterium¹, MARCUS KNUDSON, Sandia National Laboratories — The past several years have seen tremendous increase in the number of identified extra-solar planetary systems. Our understanding of the formation of these systems is tied to our understanding of the internal structure of these exoplanets, which in turn rely upon equations of state of light elements and compounds such as water and hydrogen. Here we present shock compression data for water with unprecedented accuracy that shows commonly used models for water in planetary modeling significantly overestimate the compressibility at conditions relevant to planetary interiors. Furthermore, we show that its behavior at these conditions, including reflectivity and isentropic response, is well described by a recent first-principles based equation of state. These findings advocate the use of this model as the standard for modeling Neptune, Uranus, and “hot Neptune” exoplanets, and should contribute to improved understanding of the interior structure of these planets and, perhaps improved understanding of formation mechanisms of planetary systems. We also present very recent experiments on deuterium that have taken advantage of continued improvements in both experimental configuration and the understanding of the quartz shock standard to obtain Hugoniot data with a significant increase in precision. These data will prove to provide a stringent test for the equation of state of hydrogen and its isotopes.

4:30PM W5.00002 Simulation of methane-water mixtures at extreme conditions, SANDRO SCAN-DOLO, The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, MAL-SOON LEE, Grand Valley State University Allendale, MI, USA, NORALDA KUMARA DE SILVA, SARAYAN ADHIKARI, Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal — Simulations and experiments carried out separately on methane and water, the main components of the middle layers of Neptune and Uranus, show that at those conditions methane disproportionate into carbon-rich species and water dissociates to form an ionic liquid. Water becomes electronically conducting only at the conditions found in the deepest layers of the planets. More recent simulations on water/methane mixtures suggest a pressure-induced softening of the methane-water intermolecular cohesion, which points to an electronically conducting mixture under extreme conditions. In the mixtures, ionized water causes the progressive ionization of methane and the mixture becomes electronically conductive at milder conditions than pure water. Calculations on the crystalline counterparts, methane hydrate clathrates, suggest however a different picture: mixtures at low temperature become increasingly unstable, with increasing pressure, towards phase separation, despite the prediction of a solid-solid phase transition between MH-III, the known high-pressure form of methane hydrate, and a new hypothetical phase.

5:45PM W5.00003 Nanodiamond formation via thermal radiation from an air shock, PAUL DE CARLI, SRI International — Nanodiamonds have recently been found in sediments of Younger Dryas age, about 12,900 years ago. Carbon isotope ratios imply that the source of carbon was terrestrial organic material and rule out the possibility that the diamond was of cosmic origin, e.g., from an influx of meteorites. The nanodiamonds are associated with mineral spherules (and other shapes) that have compositions and textures consistent with the rapid melting and solidification of local soil. The inferred temperatures are much too high for natural events such as forest fires. Similar deposits of nanodiamond have been found in the 65 million year old K-Pg layer associated with the ca. 200 km diameter Chicxulub impact crater. Nanodiamond have also been reported in the vicinity of the Tunguska event, presumed to be the result of an air shock produced by the interaction of a rapidly moving cosmic body with the Earth’s atmosphere. We infer that the nanodiamonds were formed when the thermal radiation from the air shock pyrolyzed surface organic matter. Rapid reaction locally depleted the atmosphere of oxygen and the remaining carbon could condense as nanodiamond. A similar mechanism can be invoked to account for the formation of nanodiamond as a product of the detonation of oxygen-deficient high explosives.

¹This research was funded by the US Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.
5:00PM W5.00004 Apophis, Earth and Moon, I.V. LOMONOSOV, IPCP RAS, A.M. KAZANTSEV, Astr. Observ. Kyev T. Shevchenko Nat. Univ. V.V. KIM, A.V. OSTRIK, IPCP RAS — The asteroid Apophis is of great potential danger for our civilization. According to results of astronomical observations and calculations, it will fly at 40000 km distance from the Earth centre withoutcollision in 2029. However, the greater risk of the projectile. For this reason, Fraunhofer EMV operates a large variety of launchers that address velocities up to ordnance velocities as single stage powder gun but which can also be operated as two-stage light gas guns achieving the range of low earth orbital velocity. Thereby for projectile masses of up to 100 g hypervelocity impact phenomena up to 7.8 km/s can be addressed. Advanced optical diagnostic techniques like microsecond video are used as commercial systems but - since impact phenomena are mostly related with debris or dust - specialized diagnostics are developed in-house like x-ray cinematography and x-ray tomography. Selected topics of the field of applied impact physics will be presented like the interesting behavior of long rods penetrating low-density materials or experimental findings at hypervelocity for this class of materials as well as new x-ray diagnostic techniques.

5:15PM W5.00005 Rocky Planet Paradox, FLORENTIN SMARANDACHE, University of New Mexico — The science tells us that a rocky body in the Solar system whose mass exceeds 3 \times 10^{21} kg should be round. The Moon is 7.3 \times 10^{22} kg, therefore its shape is round. But the Moon rotates around the Earth. If this is the case, it is rotationally deformed to a prolate spheroid since the Moon's radius which is parallel to the trajectory is unchanged while the Moon's radius in the direction of the motion should get contracted. Yet, although the Moon orbits the Earth for geological time, it is not flat! In general, let's consider a rocky non-rotating cosmic body, with mass exceeding 3 \times 10^{21} kg that orbits the Sun or one of the solar planets. The larger is the cosmic body's orbit, the simpler is to get a small part of its orbit that looks linear. Then this cosmic body should flatten in the direction of motion, according to the Theory of Relativity, but this is in contradiction to the previous science law that this cosmic body should be round.

5:30PM W5.00006 Gravitational Collapse of Small Cores in Two-Phase Celestial Bodies, MICHAEL GRINFELD, The U.S. Army Research Laboratory, AFG, PAVEL GRINFELD, Mathematics Department, Drexel University, Philadelphia, PA — The phenomenon of gravitational collapse (GC) is well-known in theoretical astro- and planetary physics. It occurs when the incompressibility of substances is unable to withstand the pressure due to gravitational forces in celestial bodies of sufficiently large mass. The GC never occurs in incompressible models – homogenous or layered. This situation changes dramatically when different incompressible layers appear to be different phases of the same chemical substance and the mass exchange between the phases can occur due to phase transformation. The possibility of destabilization in such system becomes realistic, as it was first discovered in the Ramsey static analysis [1,2]. We will present our generalization of the Ramsey's results using dynamic approach.


5:45PM W5.00007 Equation of State of Ammonia, ROBERTA MULFORD, Los Alamos National Laboratory, SEBASTIEN HAMEL, DAMIAN SWIFT, Lawrence Livermore National Laboratory — Ammonia and water are critical components of extraterrestrial bodies, determining the density and physical properties of the Outer Planets, their moons and of extrasolar planets. Several EOS are presented for ammonia and for mixtures of ammonia, water, and methane and their properties discussed, and compared with quantum molecular dynamics predictions of the properties and evolving compositions of these mixtures as pressure and temperatures become extreme. The NH₂OH hydrate of ammonia is known to exist as a separate molecular species at pressures above about 5 GPa, and an effort is made to include reaction between NH₃ and H₂O in the description of effective EOS for mixtures. A thermodynamically complete quasiharmonic EOS for ammonia is constructed, taking into account the vibrational state splitting by molecular inversion, in determination of the heat capacity. The EOS obtained are intended for application in mass-radius relations which bound the possible interpretations of composition and structure for extraterrestrial bodies of unknown composition, in particular exoplanets.

Thursday, July 11, 2013 4:00PM - 5:45PM – Session W6 ME.5 Ballistics I Cascade II - Joshua Felts, Naval Surface Warfare Center - Indian Head

4:00PM W6.00001 Numerical Study of Liner Modification Methods Leading to Fin-stabilized Explosively Formed Penetrators, NIKOLAY ASMOLOVSKIY, VLADIMIR BASKAKOV, Bauman Moscow State Technical University — One of the methods of increasing aerodynamic properties of elongated explosively formed penetrators (EFP) is inducing fins in the rear part of the projectile. In this work a set of fins generation methods was examined. Analysis showed that small amplitude wave-shaped imperfections in circumferential area of the liner provide projectile with desired finned shape without significant changes in formation process, which can reduce development cycle compared to axisymmetric EFP. Three methods of fins generation based on imperfections induced in liner were simulated numerically using commercial software. Suitable simulation technique was chosen and modified in order to treat geometrical imperfections of small amplitudes without large computational efforts. The relation between imperfection amplitude and projectile shape was obtained. It was shown that periodic nonuniform thickness is effective method of fins generation. For example, imperfection amplitude of 2% leads to fins with amplitude 10%. Material damage properties were taken into account and yielded range of acceptable imperfection amplitude.

4:15PM W6.00002 Deformation quantification during impact testing of mild steel for velocities of 1 to 3 km/s, JAMES D. HOGAN, ROBERT J. ROGERS, JOHN G. SPRAY, University of New Brunswick, Canada — Understanding the high rate deformation of metals during hypervelocity impact is important in mitigating damage in shielding systems. Well characterized experiments are needed to improve, validate and provide reference for numerical design of these complex systems. To better understand the high rate failure of metals, this work examines the response of mild steel plates during hypervelocity impact. An electromagnetic railgun at the French-German Research Institute of Saint-Louis, France, was used as the launch platform for impact velocities of 1 to 3 km/s. The targets were 50 mm thick. Image analysis of the highly deformed pearlite grains indicates that strains upwards of 100% occur prior to failure near the impact point. Strain values decrease and grain orientations gradually change from aligned in the shock direction to random away from the impact site. Electron backscatter diffraction is used to quantify micro-structural deformation, and localized thermal and fracture effects are characterized with secondary electron microscopy.

3 This work is partially funded through the Canadian Natural Science and Engineering Research Council PGS D scholarship and the student scholarship for the APS-SCCM/AIRAPT.

4:30PM W6.00003 Applied Impact Physics Research, MATTHIAS WICKERT, Fraunhofer EMV — Applied impact physics research is based on the capability to examine impact processes for a wide range of impact conditions with respect to velocity as well as mass and shape of the projectile. For this reason, Fraunhofer EMV operates a large variety of launchers that address velocities up to ordnance velocities as single stage powder gun but which can also be operated as two-stage light gas guns achieving the range of low earth orbital velocity. Thereby for projectile masses of up to 100 g hypervelocity impact phenomena up to 7.8 km/s can be addressed. Advanced optical diagnostic techniques like microsecond video are used as commercial systems but - since impact phenomena are mostly related with debris or dust - specialized diagnostics are developed in-house like x-ray cinematography and x-ray tomography. Selected topics of the field of applied impact physics will be presented like the interesting behavior of long rods penetrating low-density materials or experimental findings at hypervelocity for this class of materials as well as new x-ray diagnostic techniques.
5:00PM W6.00004 Strength effects in an imploding cylinder with constant mass-to-explosive loading, MATTHEW SERGE, OREN PETEL, JASON LOISEAU, ANDREW HIGGINS, McGill University — High explosives were used to implode thin-walled metal cylinders of different strengths (6061-T6, 6061-T6, mild steel, and stainless steel) at a constant mass-to-explosive (M/C) ratio. The velocity history of the inner surface of the imploding cylinder was recorded via Photonic Doppler Velocimetry (PDV). The time histories and peak velocities were compared to imploding Gurney models and LS-DYNA hydrocode simulations. A model for the acceleration of the wall using a detonation pressure-based time constant gave good agreement with both the experiments and simulations. The deceleration caused by strength effects was modeled from high-strain rate theory and was used to predict the entire velocity history.

5:15PM W6.00005 Influence of the multilayer coating obtained by the HVOF method on behavior of the steel barrier at dynamic loading, PAVEL RADCHENKO, ANDREY RADCHENKO, STANISLAS BATUEV, Tomsk State University of Architecture and Building — The high velocity (supersonic) oxy-fuel (HVOF) thermal spray technology is a rather recent addition to family of thermal spray processes. This technique is considered most modern of technologies of spraying. The increase in velocity of the particles at lower temperatures allowed reducing level of oxidation of the particles and to increase the density of a powder coating. In HVOF dry dusting applicators of the first and second generations was used the cylindrical nozzle, whereas in the third generation expanding Laval nozzles are used. This method allows the velocity of a gas flow to exceed to 2000 m/sec, and the velocities of the powder particles 800 m/sec. Recently many results on elastic and strength properties of the multilayer coatings obtained by supersonic flame spraying method are received. But the main part of works on research of the coating obtained by the HVOF method is devoted to research of their stress-strain state at static loading. In this work the behavior of the steel barrier with the multilayer coating applied by HVOF is researched, at dynamic loading of projectile structure at different velocities of interaction. The problem was solved numerically within Lagrangian approach, a finite element method with the use of the explicit finite difference scheme of G. Johnson.

5:30PM W6.00006 The strength of reinforced concrete constructions under dynamic loads, ANDREY RADCHENKO, PAVEL RADCHENKO, STANISLAV BATUEV, MAXIM GONCHAROV, IGOR BALDIN, VASILIY PLEVKO, Tomsk State University of Architecture and Building — At projection of industrial and civil facilities it is necessary to consider probable dynamic loads: impact, seismic waves, etc. Results of the coordinated experimental and numerical investigations of destruction of various types of ferroconcrete elements of constructions at impact loads are given in the work.

Thursday, July 11, 2013 4:00PM - 6:00PM –
Session W7 CM.1 Equation of State: Metals Grand Crescent - Scott Crockett, Los Alamos National Laboratory

4:00PM W7.00001 Measurement of the Principal Quasi-Isentrope of Lead to ~3Mbar using the “Z” Machine, STEPHEN ROTHMAN, AWE Aldermaston, JEAN-PAUL DAVIS, MARCUS KNUDSON, TOM AO, Sandia National Laboratories, STEPHEN GOODING, AWE Aldermaston — We have measured the principal quasi-isentrope of pure lead to ~3 Mbar, using magnetically-driven ramp compression on SNL’s ‘Z’ machine. Multiple point-VISARs were used to measure the surface velocities of the compressed samples, and iterative Lagrangian analysis was used to find the wave speed as a function of ramp velocity to an accuracy of <2%. This was then integrated to longitudinal stress as a function of volume on the quasi-isentrope. The experiment used a stripped configuration with samples arranged in pairs at each of 4 vertical positions on opposite drive panels; three of the four pair positions held two lead samples of different thicknesses, while the fourth consisted of one lead sample and a bare panel for drive measurement. The thicker samples of the 3 pairs experienced weak shocks at low stress so their quasi-isentrope data is unreliable there. The single-sample data was good at low stress but affected at high stress by either effects of closure of the stripline gap and / or reflections of the compression pulse from the drive-panel rear surfaces. Data from both methods overlapped at intermediate stresses so have been combined to give the required quasi-isentrope data.

4:15PM W7.00002 Tantalum on Warm Quasi-Isentropes1, JEFFREY NGUYEN, JONATHAN BELOF, DANIEL ORLIKOWSKI, NEIL HOLMES, Lawrence Livermore National Laboratory, LAWRENCE LIVERMORE NATIONAL LABORATORY TEAM — We recently carried out a series of light-gas gun experiments to study the equation of state of tantalum along warm quasi-isentropes at up to pressures above 4 Mbars. The experiments were carried out with the use of Graded Density Impactors, which allow us to access phase space regions not previously accessible. The results are consistent with calculations. We present here equation of state data of tantalum up to 5 megabars on an elevated quasi-isentrope. The data are taken on isentropes initiating from shock Hugoniot, and thus taken a significantly different path than that of the principal isentropes. Graded density impactors were used to as pressure drivers in two-stage light gas-gun experiments. The results are consistent with calculations for the elevated isentropes.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

4:30PM W7.00003 Shock-Ramp Loading of Tin and Aluminum1, CHRISSOPHER SEAGLE, JEAN PAUL DAVIS, MATTHEW MARTIN, HEATH HANSHAW, Sandia National Laboratories — Equation of state properties for materials off the principle Hugoniot and isentrope are currently poorly constrained. The ability to directly probe regions of phase space between the Hugoniot and isentrope under dynamic loading will greatly improve our ability to constrain equation of state properties under a variety of conditions and study otherwise inaccessible phase transitions. We have developed a technique at Sandia’s Z accelerator to send a steady shock wave through a material under test, and subsequently ramp compress from the Hugoniot state. The shock-ramp experimental platform results in a unique loading path and enables probing of equation of state properties in regions of phase space otherwise difficult to access in dynamic experiments. A two-point minimization technique has been developed for the analysis of shock-ramp velocity data. The technique correctly accounts for the “initial” Hugoniot density of the material under test before the ramp wave arrives. Elevated quasi-isentropes have been measured for solid aluminum up to 1.4 Mbar and liquid tin up to 1.1 Mbar using the shock ramp technique. These experiments and the analysis of the resulting velocity profiles will be discussed.

1Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL850.

4:45PM W7.00004 ABSTRACT WITHDRAWN —
8:00AM X1.00001 What simulation can tell us about dense hydrogen, DAVID CEPERLEY, —

Friday, July 12, 2013 9:15AM - 10:45AM —
Session Y1 Plenary Session V Grand Ballroom I - Gilbert Collins, Lawrence Livermore National Laboratory

9:15AM Y1.00001 ABSTRACT WITHDRAWN —

9:30AM Y1.00002 Modeling Small-Scale Damage Experiments with TEPla , ANN KAUL, Los Alamos National Laboratory — Small-scale experiment simulations provide both focused model validation and parameter value development. Material response to loading is a complex mixture of simultaneously occurring processes such as hardening, melting and failure. The work presented here concentrates on the TEPla model of ductile failure development and evolution. Simulation results for two small-scale experiments are presented. A biaxial loading experiment is described in “Plastic Deformation and Fracture of Steels Under Dynamic Biaxial Loading” (C.K. Syn, et al., UCRL-CONF-205148). A gas-gun driven flyer plate impacts a buffer plate. The generated non-planar shock is transmitted through the buffer into a target plate, which is very thin in comparison to its diameter. The result is a biaxial tensile load which causes the target to stretch and fracture and provides a non-uniaxial test of TEPla. The RDamage experimental series studies damage initiation and fracture followed by spall layer recollection (A.M. Kaui, et al., Proc. APS-SCCM-2009). An electromagnetically-driven cylindrical shell impacts a cylindrical target shell, producing a failure surface and released spall layer. An extended EM drive allows recollection of this layer. Simulation tests parameter values for development and crush-out of porosity.
9:45AM Y1.00003 Deformation behavior of a Ce-Al bulk metallic glass. LAURA CHEN, DANIEL EAKINS, Imperial College London, NARESH THADHANI, Georgia Institute of Technology, DAMIAN SWIFT, MUKUL KUMAR, Lawrence Livermore National Laboratory — The mechanisms of stress relaxation in metallic glasses under high strain rates are an area of active study. The lack of extended structure forces strain accommodation through alternative modes to slip. For example, amorphous Ce$_2$Al has been shown to undergo a phase transition to the crystalline FCC Ce$_2$Al at 25 GPa under quasistatic loading. Whether this mechanism extends to high strain rates has yet to be determined. We present results of an initial study into the ultimate test deformation characteristics of a Ce-Al bulk metallic glass. Using the Janus laser at the Jupiter Laser Facility (LLNL), thin targets ~30 µm in thickness were shocked over a range of pressures up to 50 GPa. The velocity of the target rear surface was measured using a line-imaging VISAR to reveal features in the wave profile attributed to stress relaxation. In addition, experiments were performed on crystalline forms of Ce-Al prepared through heat treatment of the amorphous material. Preliminary results reveal a distinct precursor wave in the amorphous material below 20 GPa, which gives way to a complex multiwave structure above 30 GPa. Results of analyses in terms of the contribution of elastic energy to Gibbs' free energy of the initial phase are also presented.

10:00AM Y1.00004 Shock Response of Bi/W Composites, KYLE SULLIVAN, DAMIAN SWIFT, MATTHEW BARHAM, JAMES STOLKEN, MUKUL KUMAR, Lawrence Livermore National Laboratory, LAWRENCE LIVERMORE NATIONAL LABORATORY TEAM — This work investigates the shock response of composite pellets, whose constituents have a widely disparate shock melting response; a low melting phase, Bi, and a high melting phase, W. Samples were mixed using low-energy ball milling, followed by uni-axial pressing with and without heating to yield a range of compositions, densities, and microstructures. Laser-driven shocks were generated in the samples, and the shocked samples were collected for post-mortem analysis. On the laser drive side, we observe craters up to several hundred micrometers deep, which presumably form as Bi is shock-melted, and material is unloaded as tensile stresses develop from the release wave interactions. We find that the depth of the crater (i.e. the melting depth) is primarily governed by the composition and sample porosity. On the spall surface, we observe various behaviors, ranging from no damage to large spall regions, depending on the composition of the sample. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

10:15AM Y1.00005 Coupling Instrumented Experiments with Microstructure-based Simulations of Reactant Configuration Effects on Shock-Initiation of Reactions in Intermetallic-Forming Powder Mixtures, NARESH THADHANI, Georgia Institute of Technology — The shock-initiation of reactions in intermetallic-forming powder mixtures is dominated by the configuration of reactants, which is influenced by the intrinsic and extrinsic properties of constituents. Instrumented experiments coupled with microstructure-based simulations can be used to understand the meso-scale processes and effects of reactant configuration on the onset conditions for reaction initiation. Uniaxial-strain impact experiments are performed to monitor the input and propagated stress-wave profiles and to determine changes in the stress history during plastic deformation and phase transformation. Laser-driven shocks were generated in the samples, and the shocked samples were collected for post-mortem analysis. The simulations reveal the dependence of the starting configuration of reactants on the heterogeneous nature of localized deformation and mixing with processes such as forced or turbulent flow, vortex formation, and dispersion of reactants, influencing the onset conditions for reaction initiation. Understanding of these processes as a function of the effects of starting reactant configuration and correlating those with synthetically-generated microstructural constructs allows reverse design of reactive powder mixture systems for desired macro-scale performance. This presentation will present an overview of our experimental and modeling approach in understanding the mechanistic aspects of impact-initiation of reactions for design of reactive materials systems.

Support provided by AFOSR, DTRA, and ONR.

Friday, July 12, 2013 9:15AM - 10:45AM — Session Y2 CM.1 Equation of State: Hydrogen

| Time  | Session Title | Speaker | Institution | Abstract
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<td>9:15AM</td>
<td>Y2.00001 LiH equation of state by static and shock compression</td>
<td>AMY LAZICKI, Lawrence Livermore National Laboratory — We will present experimental progress towards a more complete picture of the equation of state of LiH at extreme conditions, for the purpose of constraining theoretical models. A high-precision 300K isotherm up to 2.5 Mbars was measured using X-ray diffraction on polycrystalline samples compressed in diamond anvil cells, revealing that LiH does not transform from the B1 phase to the predicted B2 phase in this pressure range. Raman spectroscopy probed the vibrational properties along the isotherm. We will also present new results from shock compression studies of the principle Hugoniot between 3 and 8 Mbars. Portions of this work were performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.</td>
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<td>9:45AM</td>
<td>Y2.00002 Hydrogen in Simple Molecular Systems under Pressure</td>
<td>GUSTAV BORSTAD, Department of Physics, Washington State University and Institute for Shock Physics, CHOONG-SHIK YOO, Department of Chemistry, Washington State University and Institute for Shock Physics — Hydrogen-rich systems are studied due to their importance in revealing fundamental properties and giving rise to novel behaviors as well as the hope of using the currently known and remarkable properties of hydrogen for applications. The hydrogen molecule (and its isotopic forms) is of interest in its own right as the simplest molecule; yet it forms an extremely complicated solid with many interesting properties observed or expected to be observed under high pressure. Furthermore, the novel behavior observed in simple binary mixtures of hydrogen and simple molecular systems, such as water, ammonia, and methane, where the mixture alters the structure and properties of both systems, giving rise to a new system different from either species alone. This provides interesting insights into the effects of the environment on these molecules and on their resulting interactions and properties. In this talk, we will present a summary of the results obtained from Raman spectroscopic studies on these systems, and we will compare and contrast the properties of these hydrogen-rich mixtures as the simple molecular species is varied.</td>
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Support provided in support of NSF-DMB (Grant No. 0854618 and 1203834).

1The work has been performed in support of NSF-DMB (Grant No. 0854618 and 1203834).

10:00AM Y2.00003 Unusual Stoichiometries of Hydrogen and Iodine Under Pressure | ANDREW SHAMP, EVA ZUREK, University at Buffalo, SUNY — Evolutionary structure searches are combined with density functional calculations to examine the most stable stoichiometries and structures of hydrogen-rich iodine phases, H$_2$I with n>1, under pressure. With respect to decomposition into hydrogen and iodine the first of the stoichiometries, H$_3$I, is predicted to become thermodynamically preferred at ~30 GPa and remain stable until H$_2$I, consisting of chains of molecular hydrogen within a iodine sublattice, becomes the global thermodynamic minimum at ~90 GPa. H$_2$I consisting of both molecular and atomic hydrogen within H$_n$-I chains is predicted to remain insulating until ~70 GPa whereas the H$_2$I stoichiometry is predicted to become metallic at ~5GPa, well before it becomes thermodynamically stable. A second metallic phase, H$_4$I, present on the convex hull at pressures above 100 GPa is constructed of a graphene-like molecular hydrogen sublattice between layers of a hexagonal iodine sublattice. |
10:15AM Y2.00004 Isotopic Studies of Hydrogen and Deuterium Phase IV at Multi-Megabar Pressures, EUGENE GREGORYZAN, CHRISTOPHE GUILLAUME, THOMAS SCHELER, ROSS HOWIE. Centre for Science at Extreme Conditions and School of Physics, University of Edinburgh — The recent discovery of the mixed atomic and molecular phase IV of hydrogen (deuterium) is exemplary of how the studies of hydrogen at multi-megabar pressures is constitutive to the understanding of simple systems at extreme compressions [1]. Through a series of high pressure Raman spectroscopic experiments we have conducted an isotopic comparison between hydrogen and deuterium in phase I. Isotopic studies not only reveal differences in phase stability, imposing constraints on the P-T phase diagram, but also provide strong evidence for structural phenomena, such as proton (deuteron) tunnelling [2,3]. New data will be presented over a wide temperature range.


10:30AM Y2.00055 The essential differences between dynamic and static compression, W.J. NELLIS, Harvard University — In 1935 Wigner and Huntington (WH) predicted that at density $D_{\text{thry}} = 0.62$ mole H/cm$^2$, “very low temperatures,” and a pressure greater than 25 GPa, bcc H$_2$ undergoes an isostuctural phase transition directly to H with an associated insulator-metal transition (IMT). In 1996 metallic fluid H was made under dynamic compression in a cross over from H$_2$ to H that completes at $D_{\text{exp}} = 0.64$ mole H/cm$^2$, 140 GPa and $T \sim 2600$ K. The Free-electron Fermi temperature $T_F = 220,000$ K and $T/T_F = 0.012 \pm 0.1$, as for ordinary metals at 300 K. To date solid metallic hydrogen has yet to be made at static pressures up to $\sim 300$ GPa at $T \sim 300$ K. This difference between electrical conductivity of H$_2$ compressed dynamically and statistically begs the question of why fluid H at 140 GPa and $\sim 300$ K becomes metallic at 0.64 mol H/cm$^2$, the density predicted by WH for their IMT at low T; whereas metallization of solid H$_2$ or H near 300 K is yet to be achieved experimentally at pressures up to $\sim 360$ GPa? The answer is systematic differences induced by the rate of application of pressure in the two methods. Slow compression at $\sim 300$ K strengthens solid H$_2$ by inducing intermolecular bonds, which impede dissociation, metallization and perhaps even thermal equilibrium. Fast dynamic compression of liquid H$_2$ up to $\sim 300$ K precludes formation of intermolecular H-H bonds, which permits fluid H$_2$ to weaken to dissociation and thus metallization at 140 GPa. Dynamic- and static-compression effects on materials will be compared in the context of how they effect metallization of hydrogen.

Friday, July 12, 2013 9:15AM - 10:45AM —
Session Y3 NT.1 Novel Techniques: Pulsed power/Magnetic Gauges

Fifth Avenue - Jeremy Danielson, Los Alamos National Laboratory

9:15AM Y3.00001 The Experimental Researching on Cylindrical Isotropic Compression by Ultrahigh Magnetic Field, ZHUOWEI GU, HAO LUO, HENGDI ZHANG, SHICHAO ZHAO, XIAOSONG TANG, YANJIN TONG, ZHENFEI SONG, FULI TAN, JIANHENG ZHAO, CHENGWEI SUN, Institute of Fluid Physics, Chinese Academy of Engineering Physics, INSTITUTE OF FLUID PHYSICS, CHINESE ACADEMY OF ENGINEERING PHYSICS TEAM — The cylindrical isometric compression by ultrahigh magnetic field (MC-I) is a kind of unique high energy density technique. It has characters like ultrahigh pressure and low temperature rising, and would have widely used in areas like high pressure physics, new material synthesis and ultrahigh magnetic field physics. The Institute of Fluid Physics, Chinese Academy of Engineering Physics (IFP, CAEP) has begun the experiment since 2011 and a primary experimental device had been set-up. In the experiments, a seed magnetic field of 5 Tesla were set-up first and compressed by a stainless steel liner which is driven by synchronous initiated high explosive. The internal diameter of the liner is 97 mm, and its thickness is 1.5 mm. The movement of liner was recorded optically and a typical turning-around character was observed. From the photograph results the liner was compressed smoothly and evenly and its average velocity was about 5-6 km/s. In the experiment a maximum axial magnetic field of 540 Tesla has been recorded and its response magnetic pressure is more than 100 GPa. The MC-1 process was numerical simulated by 1D MHD code MC11D and the simulations was compressed smoothly and evenly and its average velocity was about 5-6 km/s. In the experiment a maximum axial magnetic field of 540 Tesla has been recorded and its response magnetic pressure is more than 100 GPa. The MC-1 process was numerical simulated by 1D MHD code MC11D and the simulations

9:30AM Y3.00002 Optical Diagnostics For High Power Pulsed Underwater Electrical Discharge Characterization, JULIEN DEREO, GILLES AVRILLAUD, Bmax, 30 bd de Thibaud, 31104, Toulouse, France, MICHEL BOUSTIE, ALAIN CLAVERIE, EKATERINA MAZANCHENKO, Institut PPRIME, CNRS-ENSMA-Universit´e de Poitiers, B.P.40109, 86960, Futuroscope, France, DAVID ASSOULIN, IDDR, RUE DE SACLY, 91128, Palaiseau, France, ALAIN BOURJADE, Aix Marseille University, 200, Avenue de Luminy, 13288, Marseille, France — We developed a simple magnetic gauge for measuring free surface velocities due to rock blasts. We considered the use of metallic flyers and barriers with the embedded particle velocity gauge technique, which is based on a magnetic field which is measured using a small detecting coil. The gauge is cheap and very simple to operate, and therefore favorable for mapping the velocity distribution at multiple points of interest on the surface.

9:45AM Y3.00003 Optical Diagnostics for High Power Pulsed Underwater Electrical Discharge Characterization, MICHAEL GOFF, GARETH APPLEBY-THOMAS, Cranfield University, MALCOLM BURNS, AWE, PAUL HAZELL, University of New South Wales, RICK GUSTAVSEN, LNL, CHRIS STENNET, Cranfield University — A number of experiments were carried out using a modified version of the standard particle velocity gauge technique in plate impact experiments with inert targets. Unusually these utilised metallic flyer plates. Traditional methodology advises against the use of metallic flyer/baybar with this technique, additional conductive objects moving in the magnetic field produce perturbations in the output gauge voltage. This body of work investigated the causes of the perturbation effect, methods of minimising its magnitude and possible post-processing correction methods. In experiments with Al flyers, perturbations on the order of 15% of signal strength were observed. While the magnitude of the voltage traces were distorted, key features such as shock impact could still be observed, and shock trackers were still effective. Mitigating techniques such as laminated flyers and were tried and reduced the perturbation effect, but adversely affected the shock input produced. The case of metallic barriers was also examined and similar effects observed. This study has indicated that while a coarse empirical correction is possible, uncertainty in the validity of the correction would preclude against the use of metallic flyers in experiments where high fidelity data is required.

10:00AM Y3.00004 Magnetic gauge for free surface velocities due to rock blasts, YECHESKEL ASHUACHA, ITAI GISSIS, CHEN AVINADAV, Rafael Advanced Defense Systems, Ltd. — We developed a simple magnetic gauge for measuring free surface velocities of rock materials in the range of 0.1-20 m/s. The gauge consists of two elements: a NdFeB magnet and a pick-up coil. The coil is attached to the free surface at the point of interest. The magnet is placed a few centimeters away from the coil on its central axis, intact from the rock. Rock surface movement due to blast loading induces current in the coil due to change of the magnetic flux. The coil velocity is deduced from the measured current using a computational code. The gauge was tested and validated in a set of free-falling experiments. We present velocity measurements from various blast experiments in limestone and reinforced concrete, using both the magnetic gauge and a Doppler interferometer. The results obtained from the two measurement techniques were in good agreement during a few milliseconds. The magnetic gauge is cheap and very simple to operate, and therefore favorable for mapping the velocity distribution at multiple points of interest on the surface.
10:15AM Y3.00005 A New Diagnostic for Shock Experiments: Pulse Correlation Reflectometry, TERRY SALTER, Los Alamos National Laboratory — Based on the conceptually simple principle of time domain reflectometry, the pulse correlation reflectometry technique allows for the determination of shock position as a function of time along a diagnostic cable. Once the electrical pulse speed of the cable is accurately known (via calibration), the current shock position may be determined by measuring the two-way transit time of an interrogation pulse reflected off the electrical short created by the crushed cable at the shock position. Due to electrical pulse dispersion within the cable, a pulse correlation analysis method is required to achieve the positional accuracy required for small-scale shock experiments. To further increase the positional accuracy, a method of multiplexing several pulses within the cable allows for more frequent interrogation of the dynamic shock front. With a high frequency pulser and a high bandwidth digitizer, this new technique can acquire far more data than typical fiducial pins, effectively providing a near continuous shock position measurement. Initial experiments along explosively driven surfaces indicate excellent agreement with pin and streak camera data, while yielding a second order of magnitude increase in data with an order of magnitude reduction in fielding time, complexity, and cost.

10:30AM Y3.00006 The method to improve accuracy and informativeness of shock-wave study of solids by means of electric explosion of foils, IVAN SMIRNOV, YURI SUDENKOV, St. Petersburg State University — The experimental technique using the phenomenon of electric explosion of foils for generation of shock waves in solids will be presented. The developed setup allows to carry out the study of deformation and fracture processes in materials under high-speed loading with the pulse duration of 0.5–1 µs and pressures up to 20 GPa. As well as for any methods of impact loading, the traditional technique of application of electric explosion of foils does not allow to register parameters of loading pulse. However the use of symmetry of the foil explosion makes it possible to register with sufficient accuracy both the initial parameters of the shock wave, and the shock wave output to the sample free surface. The results of application of such technique in studies of elastic-plastic processes and spall strength of metals will be shown.

Friday, July 12, 2013 9:15AM - 10:15AM — Session Y4 TM Continuum Modeling IV  Vashon - Tim Germann, Los Alamos National Laboratory

9:15AM Y4.00001 Combined Hydrodynamic and Diffraction Simulations of Femtosecond X-Ray Scattering from Laser-Driven Crystals, JUSTIN WARK, ANDREW HIGGINBOTHAM, University of Oxford, DESPINA MILATHIANAKI, LCLS, SLAC, ARIANNA GLEASON, Stanford University — We describe a simple hydrocode based on a two-step integration scheme that models the evolution of elastic and plastic strains in crystals subject to rapid laser-shock loading. By monitoring the elastic strains during plastic flow we track the rotation and spacing of lattice planes within the polycrystalline sample, and can thus predict the signal that would be produced by X-ray diffraction in a variety of experimental geometries. By employing a simple Taylor-Crowl dislocation model we simulate diffraction patterns from in a Debye-Scherrer geometry to track the orthogonal strain states within a laser-shocked sample. The yield rate is approximately matched to those observed in multi-million atom MD simulations, allowing movies to be made of the diffraction images that would be seen in a real experimental geometry, and illustrating the pertinent experimental requirements, including target texture. Judicious choice of geometry allows clear demarcation of the initial elastic response of the target to be made from the subsequent plastic relaxation. We discuss the simulations in the context of the novel experimental capabilities that have recently become available with the advent of 4th generation light sources, which allow single-shot diffraction with sub-100-fs resolution.

9:30AM Y4.00002 Modelling of the Pele Fragmentation Dynamics, JIMMY VERRELAULT, TNO — The Penetrator with Enhanced Lateral Effect (PELE) is a type of explosive-free projectile that undergoes radial fragmentation upon an impact with a target plate. This type of projectile is composed of a brittle cylindrical shell (the jacket) filled in its core with a material characterized with a large Poisson’s ratio. Upon impact with a target, the axial compression causes the filling to expand in the radial direction. However, due to the brittleness of the jacket material, very little radial deformation can occur which causes a radial stress between the two materials and a hoop stress in the jacket. Fragmentation of the jacket occurs if the hoop stress exceeds the material’s ultimate stress. The PELE fragmentation dynamics is explored via Finite-Element Method (FEM) simulations using the AUTODYN explicit dynamics hydrocode. The numerical results are compared with an analytical model based on wave interactions, as well as with the experimental investigation of Paulus and Schirm (1996). The comparison is based on the mechanical stress in the filling, the resulting radial velocity of the fragments, the number of fragments generated and their mass distribution.

9:45AM Y4.00003 On the scaling of the magnetically accelerated flyer plate technique to currents greater than 20 MA, R.W. LEMKE, M.D. KNUDSON, K. COCHRANE, M.P. DESJARLAIS, J.R. ASAY, Sandia National Laboratories — In this talk we discuss scaling the magnetically accelerated flyer plate technique to currents greater than are available on the Z accelerator. Peak flyer plate speeds in the range 7–46 km/s are achieved in pulsed power driven, hypervelocity impact experiments on Z for peak currents in the range 8–19 MA. The highest (lowest) speeds are produced using aluminum (aluminum-copper) flyer plates. In either case, the ~1 mm thick flyer plate is shocklessly accelerated by magnetic pressure to ballistic speed in ~400 ns; it arrives at the target with a fraction of material at standard density. During acceleration a melt front, due to resistive heating, moves from the drive-side toward the target-side of the flyer plate. The speed of the melt front increases with increasing current. Peak flyer speeds on Z scale quadratically (linearly) with current at the low (high) end of the range. Magnetohydrodynamic simulation shows that the change in scaling is due to geometric deformation, and that linear scaling continues as current increases. However, the combined effects of shockless acceleration and resistive heating lead to an upper bound on the magnetic field feasible for pulsed power driven flyer plate experiments, which limits the maximum possible speed of a useful flyer plate to <100 km/s.

1 Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corp., a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Dept. of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:00AM Y4.00004 Generation of isentropic compression by use of multi-layer composite flyer and its influence on system thermodynamics: A simulation study, ADITI RAY, Bhabha Atomic Research Centre, Mumbai, India — Recently the possibility of achieving quasi-isentropic compression using functionally graded materials, in both gas gun and explosive driven systems was explored by hydrodynamic simulations. In the current paper, we show that multi-layered composite flyer with progressively increasing shock impedances, referred to as graded density impactor (GDI), has the potential to carry out the study of deformation and fracture processes in materials under high-speed loading with the pulse duration of 0.5–1 µs and pressures up to 20 GPa. As well as for any methods of impact loading, the traditional technique of application of electric explosion of foils does not allow to register parameters of loading pulse. However the use of symmetry of the foil explosion makes it possible to register with sufficient accuracy both the initial parameters of the shock wave, and the shock wave output to the sample free surface. The results of application of such technique in studies of elastic-plastic processes and spall strength of metals will be shown.
9:15AM Y5.00001 Novel Small-scale Technique for Determining Detonation Velocity, DANIEL PRESTON, LARRY HILL, BRYCE TAPPAN, LANL — Measuring the local detonation velocity of an explosive has been limited to rate stick and cylinder tests. These tests traditionally used break wires, pins, and more recently PDV as a velocity diagnostic. These experimental techniques can be very accurate at measuring detonation velocities but are costly and require tens to hundreds of grams of material. This paper presents a novel small-scale technique for inferring detonation velocity from a modest sized pellet of explosive. A streak image is taken of the breakout shock on the flat output side of the pellet. Assuming a spherical shock wave, one can show that the breakout trace is of hyperbolic form. From this, one can simultaneously infer detonation velocity and apparent center. This method is ideal for energetic formulation and synthesis development due to the small amount of material required. Furthermore, this paper discusses the accuracy and limitations of this technique.

9:30AM Y5.00002 Computer Simulations to Study the Effects of Explosive and Confinement Properties on the Deflagration to Detonation Transition (DDT)

9:45AM Y5.00003 A view on the functioning mechanism of EBW detonation - Part 2: Exploding Bridgewire Output

10:00AM Y5.00004 Review of the concept and of the equations of the weldability window for explosive welding. Application to the explosive welding of stainless steel to carbon steel in cylindrical configuration

1 JER's activity was performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344, and partially funded by the Joint US DoD/DOE Munitions Technology Development Program.

9:15AM Y6.00001 A Multiphase Approach for Modeling the Shock Response of Unidirectional Composite Materials, SHANE SCHUMACHER, Sandia National Laboratories, CHRIS KEY, HI Test Laboratories, KEVIN RUGGIRELLO, SCOTT ALEXANDER, Sandia National Laboratories — The shock response of unidirectional fiber reinforced composite materials is inherently anisotropic due to their microstructural geometric configuration. Unlike typical elastic-plastic materials, composite materials form the observed two-wave structure under longitudinal shocks due to a precursor wave travelling through the fibers ahead of a bulk wave in the resin constituent. The nature of this response presents a problem in traditional hydrocode frameworks where each cell or material point tracks only a single velocity field. This paper outlines an adaptation of the Baer and Nunziato multi-phase model in CTH where a mixture rule is used to determine the velocity field of each constituent (fiber and matrix) of the composite material. The model modifies the momentum exchange term to represent the frictional drag forces between the fiber and matrix constituents, while assuming no mass or energy exchange. The momentum drag model is dependent not only upon the pressure difference between the constituents but also the directional dependence of the shock response. Finally, the model is implemented and compared to experimental data.
9:30AM Y6.00002 The use of lateral gauges in the assessment of shear strength in a carbon fibre composite. DAVID WOOD, GARETH APPLEBY-THOMAS, MICHAEL GOFF, Cranfield University, NICHOLAS BARNES, AWE, PAUL HAZELL. The University of New South Wales, JAMES WILGEROTH, Imperial College London — Laterally orientated manganin stress gauges have been used in obtaining the strength measurements in multiple materials, most commonly polymers and metals. Composites such as carbon fibre provide an interesting challenge for lateral gauges as any long range order within the composite will be broken up by the inclusion of the gauge. This study has investigated the shear strength of multiple orientation of a carbon fibre composite (TWCP) also compared with the matrix material of the composite investigated alone. From this data it can be ascertained whether the lateral gauge technique of measuring lateral strength is appropriate for composites with long range order.

9:45AM Y6.00003 Improved understanding of the dynamic response in anisotropic directional composite materials through the combination of experiments and modeling1, C.S. ALEXANDER, Sandia National Laboratories — Recently there has been renewed interest in the dynamic response of composite materials; specifically low density epoxy resin binders strengthened with continuous reinforcing fibers. This is in part due to the widespread use of carbon fiber composites in military, commercial, industrial, and aerospace applications. The design community requires better understanding of these materials in order to make full use of their unique properties. Experimental testing has been performed on a unidirectional carbon fiber - epoxy composite, engineered to have high uniformity and low porosity. Planar impact testing was performed at the Shock Thermodynamics Applied Research (STAR) facility at Sandia National Labs resulting in pressures up to 15 GPa in the composite material. Results illustrate the anisotropic nature of the response under shock loading. Along the fiber direction, a two-wave structure similar to typical elastic-plastic response is observed, however, when shocked transverse to the fibers, only a single bulk shock wave is detected. The two-wave structure persists when impact occurs at angles up to 45 degrees off the fiber direction. At higher pressures, the epoxy matrix dissociates resulting in a loss of anisotropy. Details of the experimental configurations and results will be presented and discussed. Greater understanding of the mechanisms responsible for the observed response has been achieved through the use of numerical modeling of the system at the micromechanical level using the CTH hydrocode. From the simulation results it is evident that the observed two-wave structure in the longitudinal fiber direction is the result of a fast moving elastic precursor wave traveling in the carbon fibers ahead of the bulk response in the epoxy resin. Similarly, in the transverse direction, results show a collapse of the resin component consistent with the experimental observation of a single shock wave traveling at speeds associated with bulk carbon. These results will be discussed within the context of the experiments and will be used to show where additional mechanisms, not fully described by the currently used models, are present.1Sandia National Labs is a multi-program laboratory managed and operated by Sandia Corp., a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:15AM Y6.00004 Development of a shock wave adhesion test for composite bonds by laser pulsed and mechanical impacts, ROMAIN ECAULT, MICHEL BOUSTIE, FABIENNE TOUCHARD, Institut PPRIME, MICHEL ARIERGONI, ENSTA - Bretagne, LAURENT BERTHE, PIMM, CNRS COLLABORATION — Evaluating the bonding quality of composite material is becoming one of the main challenges faced by aeronautical industries. This work aims the development of a technique using shock wave, which would enable to quantify the bonding mechanical quality. Laser shock experiments were carried out. This technique enables high tensile stress generation in the thickness of composite bond without any mechanical contact. The resulting damage has been quantified using different method such as confocal microscopy, ultrasound and cross section observation. The discrimination between a correct bond and a weak bond was possible thanks to these experiments. Nevertheless, laser sources are not well adapted for optimization of such a test since it has often fixed parameters. That is why mechanical impacts bonded composites were also performed in this work. By changing the thickness of aluminum projectiles, the tensile stresses generated by the shock wave propagation were moved toward the composite/bond interface. The observations made prove that the key parameters for the development of a bonding test using shock wave have been identified.

10:30AM Y6.00005 Shock responses of graphene reinforced composites via molecular dynamics simulations, HAILIN SHANG, WENQIANG WANG, Laboratory for Shock Wave and Detonation Physics, Institute of Fluid Physics, China Academy of Engineering Physics — Shock responses of graphene reinforced composites are investigated using molecular dynamics simulations. The first case studied is the response of spaced multilayer graphene plates under normal impact of a spherical projectile, focusing on the effect of the number of graphene monolayers per plate on the penetration resistance of the armor. The simulation results indicate that the penetration resistance increases with decreasing number of graphene monolayers per plate. The second case studied is the penetration resistance of laminated copper/graphene composites. The simulation results demonstrate that under normal impact by a spherical projectile the penetration resistance of copper can be improved significantly by laminating the copper plates with graphene. And the influence of graphene on the formation and growth of adiabatic shear bands in copper/graphene composites has also been discussed. The results of this research have revealed the possibility that graphene be used in the armor systems to enhance their penetration resistance.


9:15AM Y7.00001 Melting Kinetic Effects in Metals Caused by a Femtosecond Laser Pulse, POLINA KRASNOVA, DMITRY MINAKOV, MIKHAIL POVARNITSYN, PAVEL LEVASHOV, KONSTANTIN KHISHCHENKO, IHNT RAS — Melting of metals induced by a femtosecond laser pulse represents a non-equilibrium process. At the initial stage of melting and medium evolution the temperature of electrons is significantly higher than that of the ions one. This difference may lead to the increasing of the crystal melting temperature, and also to more complex relations between the temperature of electrons and ions and the transport coefficients (permittivity, thermal conductivity, electron-ion exchange). We have investigated the influence of these effects on the temperature of electrons and ions of an aluminum target using the two-temperature model. A simple kinetic model based on the evaluation of the overheated crystal lifetime was used. We estimated the increasing of the melting temperature by means of quasi-harmonic model and Lindemann criterion, and the equation of state for electrons and spinodal parameters of the crystals by means of numerical modeling using DFT and quantum molecular dynamics. The equation of state for ions is semiempirical. We provided the analysis of kinetic effects of melting of an aluminum target induced by a femtosecond laser pulse for variety of intensities.
9:30AM Y7.00002 The effect of in-situ high-temperature high-pressure on the structural changes of single-crystal relaxor ferroelectrics PbSc1/2Ta1/2O3 (PST) and PbSc1/2Nb1/2O3 (PSN) .
NAEMI WAESELMANN1, BORIANA MIHAIOVA, Universität Hamburg, Germany, MARIN GOSPODINOV, Bulgarian Academy of Sciences, Sofia, Bulgaria, ULLRICH BISMAYER, Universität Hamburg, Germany — Relaxor ferroelectrics (relaxor) of the perovskite structure (ABO3) have remarkably high dielectric permittivity dependent on temperature and frequency as well as remarkable piezoelectric and electro-optic coefficients. These structurally heterogeneous materials undergo a sequence of structural changes on the mesoscopic scale associated with characteristic temperatures resulting from the development of polar order on temperature decrease. Pressure increase on the other hand favors antiferrodistortive order at room temperature. To explore the importance of the antiferrodistortive coupling on the development of polar order simultaneous high-temperature high-pressure Raman studies were undertaken on single crystals of PST and PSN from 400 – 600 K over pressures extending to 9 GPa. We find that the first pressure-induced transition R1 decreases with temperature while the second transition R2 is relatively temperature independent. The behavior of R1 is interpreted as a weakening of the polar coupling, which in turn facilitates the evolution of the preexisting medium-range antiferrodistortive order into a long-range order. The near constant value of R2 suggests that it is independent of the state of polar coupling and is mainly related to the initial correlation length of antiferrodistortive order. Thus the coexistence of both polar order and antiferrodistortive order is required for the occurrence of the relaxor state.

1 Now at: University of Washington,

9:45AM Y7.00003 Brightness Temperature and Physical-Chemical Transformation of Epoxy Resin under Shock Compression . SERGEY A. BORDZILOVSKII, SERGEY M. KARAKHANOV, LIH SB RAS, Novosibirsk, Russia, KONSTANTIN V. KHISHCHENKO, JHIT RAS, Moscow, Russia — The interest in properties of polymers at high pressure and temperature arises from their applications as structural materials in shock-wave experiments. In particular, the optical characteristics of some polymers make it possible to use those as window materials in pyrometric measurements and in VISAR technique. In the present work, we investigate the spectral radius, which is registered in the direction of shock propagation through the epoxy EC141NF samples loaded to the pressure in the range from 19 to 42 GPa. The brightness temperature of the shocked epoxy EC141NF was measured by the optical pyrometer. Experimental points are in agreement with equation-of-state results within the limits of the error. The conclusion about the absence of the chemical transformation in the epoxy at the pressure 22.5 GPa during the observation time was drawn basing on the registered particle velocity profiles.

10:00AM Y7.00004 Effect of pressure on band structure properties of Zinc Chalcogenides1 . DHARMBIR SINGH, PIET, Samalkha, Panipat, India — The first principal calculations have been carried out to study the effect of pressure on band structure of Zinc Chalcogenides. The tight-binding linear muffin-tin orbital method (TB-LMTO) within local density approximation (LDA) has been used to study the band structure properties at ambient and high pressure. The phase stability is determined from the total energy calculations within the atomic-sphere approximation (ASA). The purely theoretical calculations show that in these materials (i) at ambient pressure, zinc blende type (B3) phase is more stable than rock salt type (B1) phase; and (ii) it exhibits a phase transition from zinc blende (B3) type to NaCl type (B1) type structure at high pressure. At further ultrahigh pressure there is phase transition from NaCl type (B1) phase to CsCl type (B2) phase. Although the calculated lattice parameter, transition pressure, volume of collapse is found to be less than the experimentally observed value, but this has been explained from the fact that the calculation has been carried out at 0 K while the experiments have been performed at room temperature. Ambient & high pressure band structural results are compared with earlier obtained similar results and explained in details.

The Author would like to thank to Director, PIET for all the motivation and support

Friday, July 12, 2013 11:00AM - 1:00PM –
Session Z1 ME.5 Ballistics II – Grand Ballroom I -

11:00AM Z1.00001 Compression, Release, and Fracture in Glass During Ballistic Impact .
MICHAEL ZELLNER, Army Research Laboratory — On hold due to security. Contact David Moore for details.

11:30AM Z1.00002 Measurement of Damage Velocities in Bullet Impacts of Transparent Armor .
CHARLES ANDERSON, RORY BIGGER, CARL WEISS, Southwest Research Institute — A series of impact experiments have been conducted to examine the response of transparent material to ballistic impact. The experiments consisted of impacting 15 mm of borosilicate glass back by 9.5 mm of Lexan. The projectile was a 0.30-cal hard steel bullet designed specifically for the experiments. Residual velocities and the residual length of the bullets (which were soft-recovered in a catch box) were measured as a function of impact velocity. High-speed imaging of the impact event and post-test analysis has permitted quantification of damage propagation and the rate of propagation. The results of several experiments are presented and compared to edge-on impact experiments that have been conducted by Strasserburger et al [1].


11:45AM Z1.00003 On the ballistic response of comminuted ceramics .
AMER HAMEED, GARETH APPLEBY-THOMAS, Cranfield University, PAUL HAZELL, University of New South Wales, DAVID WOOD, Cranfield University — Recent results have strongly suggested that the ballistic-resistance of different comminuted ceramics is similar, independent of the original strength of the material. In particular, experimental work focused on the ballistic response of such materials has suggested that ballistic response is largely controlled by shattered material morphology. Consequently, it has been postulated that control of the nature of ceramic fragmentation should provide a potential route to optimise post-impact ballistic resistance. In particular, such an approach would open up a route to control in multi-hit capabilities. In this study ballistic tests into pre-formed “fragmented-ceramic” analogues assembled from compacted alumina powders with two differing morphologies were conducted. These results strongly suggested that careful choice of initial ceramic morphology should provide a route to tailor post-impact ceramic properties.

12:00PM Z1.00004 Influence of cavitator shape on projectile penetration process in soil media .
ANNA DAURSKIKH, VLADISLAV VELDANOV, Bauman Moscow State Technical University — Standoff pins (cavitators) with smaller diameter than the projectile can be used to reduce the drag during the motion in soil media due to formation of a cavity. Cavity geometry is defined by the cavitator shape, its material and environmental conditions. Combination of these factors was investigated numerically, and influence of the cavitator shape on the projectile deceleration was studied. In particular, velocities up to 1000 m/s and different angles of attack were considered. Features of projectile stability and its interaction with the walls of the cavity were examined. Additionally, experimental investigations were carried out.
12:15PM Z1.00005 Modeling the fragmentation of hypervelocity impacts on a two wall shield, JOSHUA MILLER, ERIC CHRISTIANSEN, NASA Johnson Space Center — Two wall spacecraft shields are a mass efficient method for countering the risk of solid particle environments for systems operating in space. In this approach the threat encounters the first of two walls and shock wave compresses upon impact. The compression heats the materials so that upon subsequent release the materials spread out over a much larger region than the initial threat making it much more likely that a subsequent wall can arrest the impact energy. It is of great importance in system survivability assessments to accurately model this process and to develop models that reasonably describe a broad range of materials and impact conditions. To this end an experimental effort with spherical projectiles of a range of materials has been conducted to greater than 10 km/s and augmented to a much broader range of impact conditions by impact simulations. From this effort a modeling approach has been developed that captures this process for use in survivability assessments. The model and its anchoring data are discussed here.

12:30PM Z1.00006 Optimum Structure of Whipple Shield against Hypervelocity Impact, MINHYUNG LEE, Sejong University — It has been known that the spacecraft protection issues against space debris or meteoroid impact damage are of great importance. Whipple shield structures (double spaced plates) have been investigated and empirical ballistic limit curve (BLCs) are developed. In this paper, we like to investigate an optimum Whipple Shield structure of fixed areal density and space. To do this, both lab-scale ballistic test and finite element simulation were adopted to examine the ballistic resistance of aluminum alloy targets. Blunt high strength steel projectiles with 12.7 mm diameter were launched by light gas gun against 3.3 mm thick aluminum alloy plates at velocity of 90 ~ 170 m/s. The ballistic limit velocity was obtained. Plugging failure and obvious structure deformation of targets were observed, and with the impact velocity increasing, the target structure deformation decrease gradually. Corresponding 2D finite element simulations were conducted by ABAQUS/EXPLICIT combined with material performance testing. Good agreement between the numerical simulations and the experimental results was found.

12:45PM Z1.00007 Perforation of Thin Aluminum Alloy Plates by Blunt Projectiles - Experimental and Numerical Investigation, GANG WEI, WEI ZHANG, Harbin Institute of Technology — Reducing the armoring weight has become a research focus in terms of armored material with the increasing requirement of the mobility and flexibility of tanks and armored vehicles in modern local wars. Due to high strength-to-density ratio, aluminum alloy has become a potential light armored material. In this study, both lab-scale ballistic test and finite element simulation were adopted to examine the ballistic resistance of aluminum alloy targets. Blunt high strength steel projectiles with 12.7 mm diameter were launched by light gas gun against 3.3 mm thick aluminum alloy plates at velocity of 90 ~ 170 m/s. The ballistic limit velocity was obtained. Plugging failure and obvious structure deformation of targets were observed, and with the impact velocity increasing, the target structure deformation decrease gradually. Corresponding 2D finite element simulations were conducted by ABAQUS/EXPLICIT combined with material performance testing. Good agreement between the numerical simulations and the experimental results was found.

Friday, July 12, 2013 11:00AM - 1:00PM – Session Z2 CM.1 Equation of State: Hydrogen II Grand Ballroom II - Eugene Gregoryanz, The University of Edinburgh

11:00AM Z2.00001 High Temperature Studies of Hydrogen and Deuterium at Extreme Pressures, ROSS HOWIE, PHILIP DALLADAY-SIMPSON, CHRISTOPHE GUILLIAME, EUGÈNE GREGORYANZ, The University of Edinburgh. GREGORYANZ ET AL. TEAM — Melting characteristics is an essential diagnostic in studying the properties of the interactions within a material as well as differences between the solid and liquid states. Hydrogen despite being a simple system displays immense complexity and rich physics when under extreme pressures [1]; therefore it is important to broaden our understanding of quantum systems by studying hydrogen in extended pressure-temperature regimes. Previous experimental data alludes to a maximum in the melting curve [2], which has major implications for the existence of a ground state liquid at higher pressures [3]. Recent experimental advances have allowed us to probe melting in a new region of pressure-temperature space previously inaccessible due to the chemical reactivity of H2. Through a series of high temperature Raman spectroscopic experiments we have investigated the melting curve of hydrogen and deuterium in excess of 1000K within the megabar range, conditions previously unattainable. This study not only will show the first experimental melting data on deuterium but also allow for much needed isotopic comparisons in the high temperature regime.


11:15AM Z2.00002 Dense Hydrogen in a New Light, RUSSELL HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington — TBD

11:30AM Z2.00003 Cold hydrogen EOS / phase diagram from DAC experiments to 300 GPa, MIKHAIL EREMETS, Max Planck Institute for Chemistry: Mainz — Two new phases of hydrogen have been discovered at room temperature [1]: phase IV above 220 GPa and phase V above 7280 GPa. In the present work we studied these phases in a wide temperature range with the aid of Raman, infrared absorption, and electrical measurements at pressures up to 340 GPa. Also, we revised the I-III phase boundary and thus have built a new phase diagram of hydrogen. In particular, we established a new triple point at the phase diagram at 208 GPa and T=308 K. Our new data further support the previous work [1] that hydrogen is semiconductor in phase IV and most likely semimetal in phase V. 1. Eremets, M.I. and I.A. Troyan, Conductive dense hydrogen. Nature Materials, 2011. 10: p. 927-931.

12:00PM Z2.00004 Multi-MBar studies of Oxygen and Hydrogen, PHILIP DALLADAY-SIMPSON, CSEC and School of Physics and Astronomy, U. of Edinburgh — The study of simple archetypal molecular systems having an electronic structure heavily altered by ultra-high compression holds the promise of major breakthroughs in our understanding of matter. Among these systems, oxygen and deuterium are of particular interest due to their abundance in the Universe. We have used optical and synchrotron x-ray diffraction techniques to probe O2 and H2 (D2) to above 300 GPa. Our study on dense oxygen more than doubles the pressure range at which it had been investigated before; the picture we observe is quite different from what was experimentally reported and predicted by theory. Our study on dense hydrogen (deuterium) reveal the appearance of a new semiconducting phase at above 220 GPa which persists up to 320 GPa - the highest pressure reached in our studies. This phase is characterized by emergence of intense, well defined low frequency Raman bands, together with the unprecedented softening of the vibron, ν1, and appearance of a secondary vibron, ν2 and slowly closing band-gap. Analysis of the Raman spectra suggests a peculiar graphene-like structure consisting of both atomic and molecular layers. For both systems we will discuss the differences in results and interpretations which currently present in the literature.
Cerium at Pressures up to 6 GPa

11:30AM Z3.00005 Laser shocks in diamond anvil cells pre-compressed to 6 GPa: Revealing the density and temperature contributions of the transition to conductive fluid hydrogen, Paul Loubeyre, Stéphanie Bryggo, CEA, Ryan Rygc, LLNL, Marius Millot, Berkeley University, Amy Lazicki, LLNL, Dylan Spaulding, Berkeley University, Peter Celliers, Jon Eggert, LLNL, Tom Boehly, LLE Rochester, Gilbert Collins, LLNL, Raymond Jeanloz, Berkeley University — The quest for metallic hydrogen at high pressures represents a longstanding problem in condensed matter physics. It seems that pressures in excess of 400 GPa are needed to observe the metallic state of crystalline hydrogen. On the other hand, electrically conductive fluid hydrogen has been observed at much lower pressures, first by gas-gun compression and subsequently by laser-shock compression of cryogenic deuterium. But the relation between conductive and metallic states of hydrogen is debated, due to the combined influence of density and temperature. When the density contribution is predominant, a first-order plasma phase transition (PPT) is expected, and can be considered to represent the metallization of dense fluid hydrogen. We revisit this question by presenting Hugoniot measurements on deuterium pre-compressed in diamond anvil cells up to 6 GPa. The temperature and density contributions to electrical conductivity can be disentangled. The prediction of ab-initio calculations is compared to our data set, and a reasonable location for expecting the PPT transition line will be discussed.

12:45PM Z3.00006 Molecular dynamics for Raman modes of high pressure phases of hydrogen, Ioan-Bogdan Magdau, Graeme John Ackland, CSEC, University of Edinburgh — We present ab initio molecular dynamics (MD) calculations of hydrogen at high temperature. We calculated the Raman spectra for phases III and IV and make direct comparison of Raman vibrations with experiment. The MD structures are sensitive to initial conditions and system size, but experimental comparison provides excellent discrimination between structures found, and enables us to explain some of the existing anomalies in the literature. Structures observed for pressure-temperature conditions of phase IV are based on layers of ordered molecules and layers of either static or freely rotating hexagonal trimers, however only two are consistent with experiment. The high temperature phase IV is a hexagonal structure with alternate layers of freely rotating hydrogen molecules, and hexagonal trimers. The low temperature phase III is similar to the C2/c structure previously proposed. These structures are qualitatively different from previous work which introduced spurious features through finite size effects. The MD properly accounts for anharmonic effects and gives much better agreement with Raman data than lattice dynamics calculation.

Friday, July 12, 2013 11:00AM - 1:00PM — Session Z3 CM Condensed Matter: Lanthanides and Actinides

Fifth Avenue - Tony Zocher, Los Alamos National Laboratory

11:00AM Z3.00001 Cerium under High Pressure (and Temperature): X-ray Diffraction and Emission, Radiography and Ultrasound, Magnus Lipp, Zsolt Jeney, HyUNCHAE Cynn, William Evans, Lawrence Livermore National Laboratory, Paul Chow, Yuming Xiao, Yoshio Kono, Curtis Kenney-Benson, Carnegie Institute of Washington — Modern experimental techniques have increased our knowledge of cerium’s unique behavior under the elements, an isostructural (fcc) volume collapse transition of 15% at room temperature from the γ- to the α-phase ending in a critical point. Our recent findings favor a Kondo Volume Collapse model, a step-wise decrease of the moment across the transition but then continuation of most of it. Simple radiography appears to tell us that both solid phases continue on in some form into the liquid. The contribution of the lattice-phonons to this transition is re-evaluated using a unique combination of several techniques eliminating any indirect / iterative procedures. This methodology provides new data about the elastic properties bridging the gap from the atomic to the meso-scale dimension. Our preliminary analysis indicates a larger contribution by the lattice phonons as very recently thought. This work was performed under the auspices of the US DOE by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. The X-ray studies were performed at HPCAT (Sector 16), APS/ANL. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

11:15AM Z3.00002 Experimental Investigation of Dynamic Compression and Spallation of Cerium at Pressures up to 6 GPa1, Alla Zubarava, Sergey Kolesnikov, Alexander Utkin, Institute of Problems of Chemical Physics SAS — In this study the experiments on one-dimensional dynamic compression of Cerium (Ce) samples to pressures of 0.5 to 6 GPa through an impact of AI flyer plates accelerated with various types of explosively driven generators were conducted. VISAR laser velocimeter was used to obtain Ce free surface velocity profiles. At pressures of about 0.5 GPa the isentropic compression wave which was blurred in time was registered instead of a usual shock wave. It was due to the anomalous compressibility of γ-phase of Ce. At pressures higher than 0.78 GPa that corresponded to γ-α-transition in Ce the two-wave configuration was observed which consisted of the similar wave of isentropic compression and the following shock jump. At the profiles obtained for experiments with thin Al flyer plates a shock rarefaction wave was clearly registered in Ce samples, the appearance of which was also due to the anomalous compressibility of γ-phase. In several samples spall phenomena were also observed. The results showed a strong dependence of the spall strength of Ce on the strain rate: at its increase by an order of magnitude (3*10^4 to 3*10^5 s^-1) the spall strength rose from 0.4 to 0.6 GPa. Authors would like to thank M.V. Zhernokletov for supplied samples.

1This work was supported by FAIR-Russia Research Center

11:30AM Z3.00003 Pressure-induced iso-structural phase transition in CeO2 above megabar pressures, Lei Liu, Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, CAEP, Wengen Yang, HPSync, Geophysical Laboratory, Carnegie Institution of Washington, Hongxing Song, Huayun Geng, Yan Bi, Jian Xu, Key Laboratory of Shock Wave and Detonation Physics, Institute of Shock Wave and Detonation Physics TEAM, HPSync TEAM — The pressure-induced structural phase transition of cerium dioxide, CeO2, has been studied by synchrotron angle X-ray diffraction technique using diamond anvil cell up to 175 GPa at room temperature. In addition to the Fm-3m to pnma structural phase transition at about 30 GPa, which was found previously, a pnma to pnma iso-structural phase transition was found above megabar pressure range. During the phase transition, the a axis of the unit cell collapses, while the b and c axis expand. However, abrupt change of the unit cell volume during the phase transition was not observed.

11:45AM Z3.00004 Neutron Diffraction and Electrical Transport Studies on Magnetic Transition in Terbium at High Pressures and Low Temperatures, Sarah Thomas, Jeffrey Montgomery, Georgiy Tsoi, Yogesh Vohra, University of Alabama at Birmingham, Samuel Weir, Lawrence Livermore National Laboratory, Christopher Tulk, Antonio Moreira dos Santos, Oak Ridge National Laboratory — Neutron diffraction and electrical transport measurements have been carried out on the heavy rare earth metal terbium at high pressures and low temperatures in order to elucidate its transition from a helical antiferromagnetic to a ferromagnetic ordered phase as a function of pressure. The electrical resistance measurements using designier diamonds show a change in slope as the temperature is lowered through the ferromagnetic Curie temperature. The temperature of the ferromagnetic transition decreases at a rate of -16.7 K/GPa till 3.6 GPa, where terbium undergoes a structural transition from hexagonal close packed (hcp) to an α-5m phase. Above this pressure, the electrical resistance measurements no longer exhibit a change in slope. In order to confirm the change in magnetic phase suggested by the electrical resistance measurements, neutron diffraction measurements were conducted at the SNAP beamline at the Oak Ridge National Laboratory. Measurements were made at pressures to 5.3 GPa and temperatures as low as 90 K. An abrupt increase in peak intensity in the neutron diffraction spectra signaled the onset of magnetic order below the Curie temperature. A magnetic phase diagram of rare earth metal terbium will be presented to 5.3 GPa and 90 K based on these studies.
12:00PM Z3.00005 Origin of the Pressure-Induced Volume Collapse in Tb1, GILBERTO FABBRIS, Argonne National Laboratory / Washington University in St. Louis, JINHYUK LIM, Washington University in St. Louis, JOSE RENATO MARDEGAN, Universidade Estadual de Campinas / Argonne National Laboratory, DANIEL HASKEL, Argonne National Laboratory, JAMES SCHILLING, Washington University in St. Louis — The mechanism responsible for the high-pressure volume collapse in most elemental rare-earth metals is still a matter of debate. Models attempting to explain this collapse include: (i) valence transition, (ii) 4f local-to-band transition (Mott-Hubbard), (iii) f-d hybridization (Kondo), and (iv) sp→d transfer. We focus on Tb metal which displays a 5% volume collapse at 53 GPa. X-ray absorption spectroscopy shows persistence of Tb’s 4f5 state across the volume collapse, excluding (i) as a mechanism. Furthermore, x-ray emission spectroscopy shows that 4f states retain their localized nature to at least 70 GPa, ruling out (ii). On the other hand, the suppression of the x-ray absorption “white line” with pressure indicates that sp→d transfer is active. To probe for Kondo interactions, the pressure dependence of the superconducting Tc in pure Y is compared to that in a Y(0.5 at% Tb) alloy. We observe a strong suppression of Tc at pressures near terbium’s volume collapse, an indication of a rapid increase of the Kondo temperature, in agreement with (iii). We argue that a Kondo model in the presence of sp→d transfer best describes the volume collapse in Tb metal.

1This work was supported by the NSF grant DMR-1104742 and CDAC through NNSA/DOE Grant No. DE-FC52-08NA28554. Work at Argonne is supported by DOE under Contract No. DE-AC-02-06CH11357.

12:15PM Z3.00006 Phase Transformation of U3O8 and Enhanced Structural Stability at Extreme Conditions1, FU XIANG ZHANG, MAIK LANG, RODNEY EWING, University of Michigan — A powder sample of β-U3O8 was pressurized at room temperature up to 37.5 GPa with a symmetric diamond anvil cell. XRD patterns clearly indicated that a phase transition occurred between 3-11 GPa. The high-pressure phase is a fluorite-like structure. The fluorite-like structure is stable up to 37.5 GPa. The high-pressure phase was then laser heated to over 1700 K in the diamond anvil cell at high pressures. No phase transition was found at high pressure/ temperature conditions, and the fluorite-like structure of U3O8 is even fully quenchable. The lattice parameter of the fluorite-like high-pressure phase is 5.425 Å at ambient conditions, which is smaller than that of the stoichiometric UO2. Previous experiments have shown that the stoichiometric uranium dioxide (UO2) is not stable at high pressure conditions and starts to transform to a cotunnite structure at ~30 GPa. When heating the sample at high pressure, the critical transition pressure is greatly reduced. However, the fluorite-like high-pressure phase of U3O8 is very stable at high pressure/high temperature conditions. The enhanced phase stability is believed to be related to the presence of extra oxygen (or U vacancies) in the structure.

1This work was supported by Materials Science of Actinides, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award No. DE-SC0001089.

12:30PM Z3.00007 Complex Structural Phase Transitions in Europium at High Pressure, RACHEL HUSBAND, INGO LOA, University of Edinburgh, MALCOLM MCMAHON, m.mcmahon@ed.ac.uk — Europium (Eu), which is divalent at ambient pressure due to its half-filled 4f electron shell, is an anomalous element in the lanthanide series, in which the majority of the elements are trivalent. Consequently, Eu does not fit in with the general trend of structural phase transitions observed in the trivalent lanthanide elements, and its behaviour is much more complex. The Eu-Iv phase, stable above 31.5 GPa, is the only known incommensurate structure in the lanthanide series1. Early spectroscopic measurements indicated that the valence of Eu increases continuously under pressure2, but a recent study concluded that Eu remains nearly divalent up to 87 GPa3. We will present the results of our x-ray diffraction studies of Eu up to a pressure of 100 GPa, well into the superconducting region. Initial structural studies were greatly complicated by the presence of two pressure-induced contaminant phases4,5, and so great care was taken to obtain ‘clean’ samples. We will report a transition to a second incommensurately-modulated phase, Eu-V, above 42 GPa. This transition is accompanied by an increase in modulation amplitudes and the appearance of higher-order satellite reflections, suggesting a complex modulation wave. This is the first pressure-induced incommensurate-incommensurate (non-host-guest) transition to be observed in the elements at high pressure. 1Husband et al. Phys. Rev. Lett. 109, 095503 (2012). 2Röhler, Physica B + C 144, 27 (1986). 3Bi et al., Phys. Rev. B. 85, 205134 (2012). 4Husband et al., J Phys Conf Ser. 377, 012030 (2012). 5Husband et al., High Press. Res. (in Press).

12:45PM Z3.00008 On structural, elastic and dynamic stability of rare earth nitrates: First principle calculations, B.D. SAHOO, K.D. JOSHI, S.C. GUPTA, Bhabha Atomic Research Centre, Mumbai, India - 400085 — The structural stability of LaN and CeN under hydrostatic compression has been analysed theoretically. For LaN the comparison of enthalpies calculated at various pressures for rocksalt type (B1), tetragonal (B10) and CsCl type (B2) structures suggests that the B1 phase will transform to B10 structure at ~20 GPa, in line with the experimental value of 22.8 GPa. Additionally, we predict the B10 to B2 phase transition at higher pressure of ~165 GPa. Similar transition sequence has been predicted for CeN also with the B1 to B10 and B10 to B2 transition pressures calculated as 53 GPa and 198 GPa, respectively. However, the static high pressure EXDXRD measurements on CeN by Olsen et al. report direct B1 to B2 phase transition at ~65 GPa. To resolve this discrepancy, we have performed lattice dynamic calculations on these structures. The phonon spectra calculated at zero pressure correctly shows B1 phase to be dynamically stable and B10 and B2 to be unstable. At 65 GPa the B1 phase becomes dynamically unstable and the B10 emerges as a dynamically stable phase whereas B2 still remains unstable, supporting theoretical finding. Further, our results are substantiated by calculated ADXRD pattern of B10 and B2 phases.

Friday, July 12, 2013 11:00AM - 12:30PM — Session Z4 TM Continuum Modeling V — Vashon - Joe Hooper, Naval Postgraduate School

11:00AM Z4.00001 Numerical and Theoretical Analysis of Plastic Response of 5A06 Aluminum Circular Plates Subjected to Underwater Explosion Loading1, PENG REN, WEI ZHANG, Harbin Institute of Technology — Dynamic response analysis of structures subjected to underwater explosion loading has been always an interesting field for researchers. Understanding the deformation and failure mechanism of simple structures plays an important role in an actual project under this kind of loading. In this paper, the deformation and failure characteristics of 5A06 aluminum circular plates were investigated computationally and theoretically. The computational study was based on a Johnson-cook material parameter mode which was obtained from several previous studies provides a good description of deformation and failure of 5A06 aluminum circular plates under underwater explosion loading. The deformation history of the clamped circular plate is recorded; the maximum deflection and the thickness reduction measurements of target plates at different radii were conducted. The computational approach provided insight into the relationship between the failure mechanism and the strength of impact wave, and a computing formulate for strain field of the specimen was derived based on the same volume principle and rigid-plastic assumption. The simulation and theoretical calculation results are in good agreement with the experiments results.

1National Natural Science Foundation of China (NO:11272057)
11:15AM Z4.00002 Instability in shocked granular gases, NICK SIRMAS, MATEI RADULESCU, University of Ottawa — Shocks in granular media, such as vertically oscillated beds, have been shown to develop instabilities. Similar jet formation has been observed in explosively dispersed granular media. In the current study, we investigate the origin of this instability. Both particle dynamics and continuum based simulations of the hydrodynamics of granular gases are investigated in the presence of shock compression. The shock waves are found to be unstable in the presence of dissipative collisions in the particle bed. The instability manifests itself as distinctive high density non-uniformities and convective rolls on the shock surface. The characteristic spacing of the non-uniformities is found to be well approximated by the characteristic relaxation length scale, which is controlled by both the shock strength and amount of energy dissipation in particle collisions. By studying the time evolution of the material undergoing the shock wave compression and further relaxation, we found that the gas develops the instability on the same time scales as the clustering instability in homogeneous gases. This confirms that the clustering instability is the dominant mechanism.

11:30AM Z4.00003 An Exact Riemann Solver for a Granular Mixture Model with Multiple Solid Components, MICHAEL CROCHET, KEITH GONTHIER, Louisiana State University — The solution of the two-phase Riemann problem is an essential component of finite-volume numerical methods applied to hyperbolic systems of multiphase model equations. These are typically used to study deflagration-to-detonation transition in energetic materials, and predict flow field structures associated with the dynamic compaction of gas–granular solid mixtures. A widely-used two-phase model has been extended recently to include an arbitrary number of solid components, which can be used to analyze the thermomechanical behavior of metallized explosives and mixtures containing multiple solid grain sizes. Although a solution to the two-phase Riemann problem has already been formulated for gamma-law equations of state, there is currently no available solution for the N-phase analogue in the literature. Here, an extension of the exact two-phase solution to systems containing multiple solid phases is developed, where each phase is governed by general, convex equations of state. The resulting Riemann solver can be used in the verification of existing numerical schemes, and also serve as a framework for the future construction of upwind, Godunov-based numerical methods. A general overview of the solver methodology is given, and three-phase example problems are considered.

11:45AM Z4.00004 Numerical Simulation of the Detonation Propagation in Silicon Carbide Shell, IGOR BALAGANSKY, ANTON TERECHOV, Novosibirsk State Technical University — Last years it was experimentally shown that in condensed high explosive charges (HE) placed in silicon carbide shell with sound velocity greater than the detonation velocity in HE, there may be observed interesting phenomena. Depending on the conditions, as an increase or decrease of the detonation velocity and pressure on the detonation front can be observed. There is also the distortion of the detonation front until the formation of a concave front. For a detailed explanation of the physical nature of the phenomenon we have provided numerical simulation of detonation wave propagation in Composition B HE charge, which was placed in silicon carbide shell. Modeling was performed with Ansys Autodyn in 2D-axis symmetry posing on an Eulerian mesh. Special attention was paid to selection of the parameters values in Lee-Tarver kinetic equation for HE and choice of constants to describe behavior of the ceramics. For comparison, also we have carried out the modeling of detonation in a completely similar assembly with brass shell. The simulation results agree well with the experimental data. In particular, in silicon carbide shell distortion of the detonation front was observed. A characteristic feature of the process is the pressure waves propagating in the direction of the axis symmetry on the back surface of the detonation front.

12:00PM Z4.00005 A Comparison of the Shock Response of the Material Point Method, KEVIN RUGGIRELLO, SHANE SCHUMACHER, Sandia National Laboratories — The Lagrangian Material Point Method (MPM) has been implemented into the Eulerian shock physics code CTH, at Sandia National Laboratories. Eulerian hydrodynamic methods are useful for large deformation problems, where “mesh tangling” typically leads to difficulties for Lagrangian methods. However, Eulerian techniques suffer from numerical diffusion due to advection, which can be problematic for many material models requiring the transport of a damage parameter or other state variables that need to remain sharp. The inclusion of the MPM in CTH allows for the accurate simulation of structural response to shock loading in a single framework. This paper presents a comparison of the shock response of the MPM to a Lagrangian, and Eulerian hydrodynamics code. All three solutions will be compared to exact analytical solutions in order to assess the accuracy of the shock response of each.

12:15PM Z4.00006 The Role of Quantum Nuclear Effects in Shock-Induced Chemistry and Colored ThermoStats for Their Efficient Description, EVAN REED, TINGTING QI, QIAN YANG, Department of Materials Science and Engineering, Stanford University — A fast methodology is described for atomistic simulations of shock-compressed materials that incorporates quantum nuclear effects in a self-consistent fashion. We introduce a modification of the multiscale shock technique (MSST) that couples to a quantum thermal bath described by a colored noise Langevin thermostat. The new approach, which we call QB-MSST, is of comparable computational cost to MSST and self-consistently, semi-classically incorporates quantum heat capacities and Bose-Einstein harmonic vibrational distributions. We study shock-compressed methane using the ReaxFF potential. We find that the self-consistent nature of the method results in the onset of chemistry at 40% lower pressure on the shock Hugoniot than observed with classical molecular dynamics. We employ new statistical and data mining methods to reveal the nature of the chemistry.

Friday, July 12, 2013 11:00AM - 1:00PM – Session Z5 GP2: Planetary II Cascade I - Dylan Spaulding, Harvard University

11:00AM Z5.00001 DFT modeling of chemistry on the Z machine, THOMAS R. MATTSSON, Sandia National Laboratories — Density Functional Theory (DFT) has proven remarkably accurate in predicting properties of matter under shock compression for a wide-range of elements and compounds: from hydrogen to xenon via water. Materials where chemistry plays a role are of particular interest for many applications. For example the deep interiors of Neptune, Uranus, and hundreds of similar exoplanets are composed of molecular ices of carbon, hydrogen, oxygen, and nitrogen at pressures of several hundred GPa and temperatures of many thousand Kelvin. High-quality thermophysical experimental data and high-fidelity simulations including chemical reaction are necessary to constrain planetary models over a large range of conditions. As examples of where chemical reactions are important, and demonstration of the high fidelity possible for these both structurally and chemically complex systems, we will discuss shock- and re-shock of liquid carbon dioxide (CO2) in the range 100 to 800 GPa, shock compression of the hydrocarbon polymers polyethylene (PE) and poly(4-methyl-1-pentene) (PMP), and finally simulations of shock compression of glow discharge polymer (GDP) including the effects of doping with germanium. Experimental results from Sandia’s Z machine have time and again validated the DFT simulations at extreme conditions and the combination of experiment and DFT provide reliable data for evaluating existing and constructing future wide-range equations of state models for molecular compounds like CO2 and polymers like PE, PMP, and GDP. Sandia National Laboratories is a multi-program national laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
loss of volatiles by vaporization of impacting planetesimals and erosion of the atmosphere during the end stage of planet formation. We propose that major
to induce substantial vaporization of the projectile. Using the collision history of growing planets from recent N-body simulations, we present estimates of the
ices. We have recently predicted equations of state (EOS) for water-methane-ammonia mixtures using quantum molecular dynamics and equilibrium chemistry
various impact speeds, as all of these may influence chemistry in the instrument’s antechamber and thus affect what ions or molecules are seen by the INMS.
strong insulator with Gd-O and Ga-O bond strengths similar to Mg-O and Si-O. We have measured optical reflectivities of shock fronts in melted Gd
produce the spherical annulus proposed to explain a dynamo that would generate the tilted magnetic fields. A mass distribution needs to be identified that is
compatible such as an ice may be vaporized, resulting in the acceleration of embedded particles of a less volatile material. The same model can be used to
in the corresponding density range. Thus, “ices”, rock, decomposed hydrogenous molecules, pure H, and Fe are probably all poor metals at conditions in the deep
Measured reflectivities are $\sim 0.1$, in reasonable agreement with optical properties of amorphous Gd-Ga-O calculated in the corresponding density range. Thus, “ices”, rock, decomposed hydrogenous molecules, pure H, and Fe are probably all poor metals at conditions in the deep
planetary interiors and thus miscible to a significant degree. A qualitative picture of the interiors with radially continuous mass distributions will be proposed.
planetary interiors and thus miscible to a significant degree. A qualitative picture of the interiors with radially continuous mass distributions will be proposed.
early Earth. We have conducted simulations of the chemical reactivity within an oxidized astrophysical icy mixture to close to equilibrium using a density functional tight binding (DFTB) approach. We observe that moderate
impact velocities are typically 1 to 4 times the escape velocity of the largest bodies (up to about 40 km/s). The collision velocities are large enough
ices. We have recently predicted equations of state (EOS) for water-methane-ammonia mixtures using quantum molecular dynamics and equilibrium chemistry
with Gd-O and Ga-O bond strengths similar to Mg-O and Si-O. We have measured optical reflectivities of shock fronts in melted Gd$_2$Ga$_2$O$_{12}$ from 0.5 to 2 TPa at the Osaka laser facility. Measured reflectivities are $\sim 0.1$, in reasonable agreement with optical properties of amorphous Gd-Ga-O calculated in the corresponding density range. Thus, “ices”, rock, decomposed hydrogenous molecules, pure H, and Fe are probably all poor metals at conditions in the deep
1This work was performed at LLNL under Contract DE-AC52-07NA27344, and was funded by the NASA Astrobiology program.
12:00PM Z5.00004 Nature of the interiors of Uranus and Neptune , WILLIAM NELLIS, Harvard University, N. OZAKI, Osaka University, R. AHUJA, Uppsala University, T. MASHIMO, Kumamoto University, M. RAMZAN, T. KAEWMARAYA, Uppsala University — Ever since the spacecraft flyby missions to Uranus and Neptune the nature of the interiors of these similar planets have been puzzles. Planetary materials are H-He: “ice,” hydrogenous molecular and ionic fluids; rock (oxides); and Fe. Measured gravitational moments cannot resolve mass distribution between 3-layer and 2-layer models, the former with sharp mass discontinuities and the latter with mass varying continuously. Also a puzzle is the material distribution that would produce the spherical annulus proposed to explain a dynamo that would generate the tilted magnetic fields. A mass distribution needs to be identified that is consistent with both the gravitational and magnetic data. If all materials become conductors then miscibility and dynamos are both possible. Gd$_2$Ga$_2$O$_{12}$ is a strong insulator with Gd-O and Ga-O bond strengths similar to Mg-O and Si-O. We have measured optical reflectivities of shock fronts in melted Gd$_2$Ga$_2$O$_{12}$ from 0.5 to 2 TPa at the Osaka laser facility. Measured reflectivities are $\sim 0.1$, in reasonable agreement with optical properties of amorphous Gd-Ga-O calculated in the corresponding density range. Thus, “ices”, rock, decomposed hydrogenous molecules, pure H, and Fe are probably all poor metals at conditions in the deep
1Harvard University, 2Osaka University, 3Uppsala University, 4Kumamoto University
12:15PM Z5.00005 Hypervelocity Impacts of Ice Grains into a Titanium Spacecraft Instrument Chamber , JAMES D. WALKER, SIDNEY CHOCRON, J. HUNTER WAITE, TIM G. B ROCKWELL, Southwest Research Institute — The Cassini spacecraft, currently in orbit around Saturn, has an Ion and Neutral Mass Spectrometer (INMS). There have been some unexpected readings of the instrument in flybys of the moon Enceladus. These flybys range from 7 to 18 km/s, and it has been suggested that ice grain impacts in the instrument could have a velocity-dependent response that influences the materials that the instrument records. To explore the physics of the impacts, computations were performed with CTH. Small ice grains (1 micron across) were impacted into a titanium alloy at a range of speeds of interest. Initial results indicate the formation of a titanium vapor plume begins at impact velocities of 16 km/s. Efforts have been made to quantify the titanium vapor and titanium solid and liquid ejecta at various impact speeds, as all of these may influence chemistry in the instrument’s antechamber and thus affect what ions or molecules are seen by the INMS.
12:30PM Z5.00006 Planetary structure and impact calculations using new mixture equations of state , A. CORREA, D.C. SWIFT, Lawrence Livermore National Laboratory, R.N. MULFORD, Los Alamos National Laboratory, S. HAMEL, Lawrence Livermore National Laboratory — Studies of the structure of icy planets and exoplanets, and of comet impacts, are hampered by limited high-pressure data on ices. We have recently predicted equations of state (EOS) for water-methane-ammonia mixtures using quantum molecular dynamics and equilibrium chemistry based on empirically-derived potentials. Here we use these EOS to predict astrophysical mass-radius relations with a firmer theoretical footing. We previously developed a hydrocode model of heterogeneous mixtures using stress and thermal equilibrium among a set of homogeneous components, with each component described by its own EOS and constitutive model. We have extended this model to treat multiphase flow more completely, by including a particle velocity for each component, drag, and the evolution of particle sizes. An externally-applied bulk acceleration from hydrodynamics induces different accelerations in each component, according to the differences in mass density. This model is suitable for simulating the dynamic loading of asteroids and comet nuclei, where one component such as an ice may be vaporized, resulting in the acceleration of embedded particles of a less volatile material. The same model can be used to simulate some aspects of planetary evolution, such as differentiation.
12:45PM Z5.00007 Volatile Loss during Collisional Growth of Planets , SARAH STEWART, SUJOY MUKHOPADHYAY, Harvard University — During the end stage of planet formation, rocky planets grow by collisions with planetary embryos and planetesimals. Impact velocities are typically 1 to 4 times the escape velocity of the largest bodies (up to about 40 km/s). The collision velocities are large enough to induce substantial vaporization of the projectile. Using the collision history of growing planets from recent N-body simulations, we present estimates of the loss of volatiles by vaporization of impacting planetesimals and erosion of the atmosphere during the end stage of planet formation. We propose that major differences in the noble gas signatures of the atmospheres of Venus, Earth and Mars are a result of the different outcomes of late impact events on each planet.
Friday, July 12, 2013 11:00AM - 12:30PM — Session Z6 ME.2 Composites and Polymers II Cascade II - Rick Gustavsen, Los Alamos National Laboratory
conductive fluid around 8000 K and 1 Mbar that progressively dissociates into an atomic dense plasma at higher pressure and temperature.

temperature Hugoniot data along with optical reflectivity in the warm dense regime up to 8 Mbar. Our data suggest that Nitrogen transforms to a polymeric system with a uniquely stable triple covalent bond. We conducted laser compression experiments of dense fluid nitrogen and obtained pressure-density-RYGG, JON H. EGGERT, PETER M. CELLIERS, GILBERT W. COLLINS, LLNL, RAYMOND JEANLOZ, UC Berkeley — Nitrogen is a prototypical molecular

index data in high pressure ice VII and solid hydrogen is evaluated. The research was performed in collaboration with Y. Liang, H. Shi, W. Yim, C.S. Zha and

assumptions underlying the EOM are examined through comparison with theoretical dielectric response functions obtained from solving the Bethe-Salpeter

University of Saskatchewan — The band gap of a material is one of the most fundamental properties. One approach to obtain energy gap information at

efforts on the non-bonded electron pairs of O.

incommensurate-like (N₂)₁₂D₂ system above 10 GPa and a non-crystalline

molecular alloys will be demonstrated. First, extended solid XeF₂ which transforms to novel two- and three-dimensional extended non-molecular phases and their

University — Novel van der Waals binary compounds, composed by two different molecular solids such as Xe and H₂, H₂ and O₂, NH₃ and H₂, and CH₄ and H₂, are understood as “molecular alloys” in terms of a changing of coordination numbers or a formation of clathrate system which are comparable to the

and chemical properties such as phase transitions, structural and electrical transition, optical changes, stiffness changes, and so on. In this presentation, three molecular alloys will be demonstrated. First, extended solid XeF₂ which transforms to novel two- and three-dimensional extended non-molecular phases and their metalization arising from a pressure-induced delocalization of non-bonded lone-pair electrons of F. Second, N₂-H₂ system which shows the presence of a novel incommensurate-like (N₂)₁₂D₂ system above 10 GPa and a non-crystalline δ-N₂-like non-crystalline solid that arises at the onset of solidification. Third, CO-D₂ system which shows small amount of D₂ stabilizes metastable polymeric CO at ambient conditions by forming O-D bonds which are playing a disproportionate effects on the non-bonded electron pairs of O.

11:30AM Z6.00003 Thin film metal thermistors with microsecond time response for shock temperature measurements of polymers, NICHOLAS TAYLOR, DAVID WILLIAMSON, ANDREW JARDINE, SMF Fracture and Shock Physics Group, Cavendish Laboratory, JJ Thomson Avenue, Cambridge, CB3 0HE, UK — Equations of state can be used to predict the relationship between pressure, volume and temperature. However, in shock physics, they are usually only constrained by experimental observations of pressure and volume. Direct observation of temperature in a shock is therefore valuable in constraining equations of state. Bloomquist and Sheikh (1980, 1981) and Rosenberg and Partom (1984) have attempted such observations in PMMA. However, their results disagree strongly above 2 GPa shock pressure. Here we present an improved fabrication technique, to examine this outstanding issue. We make use of the fact that the electrical resistivity of most metals is a known function of both pressure and temperature. If the change in resistance of a thin metal thermistor gauge is measured during a shock experiment of known pressure, the temperature can be calculated directly. The time response is limited by the time taken for the gauge to reach thermal equilibrium with the medium in which it is embedded. Gold gauges of thickness up to 200 nm have been produced by evaporation, and fully embedded in PMMA. These reach thermal equilibrium with the host material in under 1 µs, allowing temperature measurement within the duration of a plate impact experiment.

11:45AM Z6.00004 Dynamic fragmentation in ductile materials / new theoretical meshfree method / multiscale modeling, MICHAEL ORTIZ, California Institute of Technology —

12:15PM Z6.00005 ABSTRACT WITHDRAWN –

Friday, July 12, 2013 11:00AM - 1:00PM – Session Z7 CH.3 Chemistry: High Pressure Structures Grand Crescent - Mario Santoro, Istituto di Fisica Applicata N. Carrara

11:00AM Z7.00001 Novel Molecular Alloys under Extreme Conditions1, MINSEOB KIM, Washington State University — Novel van der Waals binary compounds, composed by two different molecular solids such as Xe and H₂, H₂ and O₂, N₃ and H₂, and CH₄ and H₂, are understood as “molecular alloys” in terms of a changing of coordination numbers or a formation of clathrate system which are comparable to the substitution or the occupation of atoms in the interstices of the host crystal lattice in metal alloy. Such molecular alloys show markedly differences in physical and chemical properties such as phase transitions, structural and electrical transition, optical changes, stiffness changes, and so on. In this presentation, three molecular alloys will be demonstrated. First, extended solid XeF₂ which transforms to novel two- and three-dimensional extended non-molecular phases and their metalization arising from a pressure-induced delocalization of non-bonded lone-pair electrons of F. Second, N₂-H₂ system which shows the presence of a novel incommensurate-like (N₂)₁₂D₂ system above 10 GPa and a non-crystalline δ-N₂-like non-crystalline solid that arises at the onset of solidification. Third, CO-D₂ system which shows small amount of D₂ stabilizes metastable polymeric CO at ambient conditions by forming O-D bonds which are playing a disproportionate effects on the non-bonded electron pairs of O.

1The work has been performed in support of the DTRA (Grant No. HDTRA1-09-1-0041 and HDTRA-12-1-0020).

11:30AM Z7.00002 Band Gap of Materials from Refractive Indices at High Pressure, JOHN TSE1, University of Saskatchewan — The band gap of a material is one of the most fundamental properties. One approach to obtain energy gap information at high pressure is to measure the reflectivity of the material in a diamond anvil cell and analyzed with the effective oscillator model (EOM). In this study, the assumptions underlying the EOM are examined through comparison with theoretical dielectric response functions obtained from solving the Bethe-Salpeter equation (BSE) and band gap energy calculated from the GW method. The validity the EOM method in the estimation of the band gap energies from refractive index data in high pressure ice VII and solid hydrogen is evaluated. The research was performed in collaboration with Y. Liang, H. Shi, W. Yim, C.S. Zha and R.J. Hemley.

1In collaboration with Yong Xue, University of Saskatchewan.

12:00PM Z7.00003 Extreme Chemistry of Warm Dense Nitrogen, MARIUS MILLLOT, UC Berkeley, J. RYGG, JON H. EGGERT, PETER M. CELLIERS, GILBERT W. COLLINS, LLNL, RAYMOND JEANLOZ, UC Berkeley — Nitrogen is a prototypical molecular system with a uniquely stable triple covalent bond. We conducted laser compression experiments of dense fluid nitrogen and obtained pressure-density-temperature Hugoniot data along with optical reflectivity in the warm dense regime up to 8 Mbar. Our data suggest that Nitrogen transforms to a polymeric conducting fluid around 8000 K and 1 Mbar that progressively dissociates into an atomic dense plasma at higher pressure and temperature.
12:15PM Z7.00004 Modeling of amorphous poly-CO structure with N and He. ISKANDER G. BATYREV, WILLIAM D. MATTSON, US Army Research Laboratory — Density functional theory simulations of amorphous poly-CO structure were performed with addition of N or He atoms to crystalline delta phase of CO. For the CO-N mixtures the concentration of N was varied in the range from 6.25% to 50% with different distribution of N atoms in the unit cell. For all studied concentrations and initial configurations, isotropic compression led to polymerization beginning at a pressure of 11 GPa. This is slightly higher than that for pure p-CO which was previously observed to start to polymerize at 8 GPa. For the nitrogen doped mixtures only the CO part of the mixtures polymerized at 11 GPa, and the N was not incorporated into the random network. For the CO-He mixtures, the concentration of He atoms in delta phase of CO was 6.25%. Formation of random networks begins at 9 GPa and at 11 GPa all CO molecules have formed a combination of closed rings and chain type structures without isolated CO molecules with a density of 2.40 g/cm³. He atoms facilitate complete formation of the random structure at lower pressure than that for pure poly-CO, which isn’t completely polymerized until compressed to a pressure of 18 GPa. He atoms also help stabilize the structure while lowering the pressure down to 100 Bar with only few CO molecules detaching in the process. Without He atoms at the same pressure there are approximately ten times the number CO molecules occupying voids in the random network.

12:30PM Z7.00005 Ammonia ice at very high pressure, SANDRA NINET, Université Pierre et Marie Curie - Institut de Mineralogie et de Physique des Milieux Condensés - Paris VI, France, FREDERIC DATCHI, Université Pierre et Marie Curie - Institut de Mineralogie et de Physique des Milieux Condensés - Paris VI, France, PAUL DUMAS, Synchrotron SOLEIL, Gif Sur Yvette, France, MOHAMED MEZOUAR, GASTON GARBARINO, European Synchrotron Radiation Facility, Grenoble, France, ADRIEN MAFETY, Université Pierre et Marie Curie - Institut de Mineralogie et de Physique des Milieux Condensés - Paris VI, France, CHRISS PICKARD, Department of Physics and Astronomy, University College London, United Kingdom, RICHARD NEEDS, Theory of Condensed Matter Group, Cavendish Laboratory, Cambridge, United Kingdom, MARCO SAITTA, Université Pierre et Marie Curie - Institut de Minéralogie et de Physique des Milieux Condensés - Paris VI, France — In this presentation, we report an extended experimental investigation of the phase diagram of ammonia at high pressure and temperature. By combining Raman scattering and X-ray diffraction experiments, we demonstrate the presence of a new H-disordered crystalline form above \( \sim 60 \text{ GPa} \) and \( \sim 700 \text{ K} \). Using \textit{ab initio} MD simulations, we show that this new disordered phase is a superionic conductor. We will also present new experimental results (infrared, Raman and X-ray) on \( \text{NH}_3 \) and \( \text{ND}_3 \) at ambient temperature up to 200 GPa and will discuss the existence of ionic ammonia ices.

12:45PM Z7.00006 The structure of ice VII on the approach to symmetrisation, MALCOLM GUTHRIE, REINHARD BOEHLER, Geophysical Laboratory, Washington, DC, USA, CHRISTOPHER TULK, ANTONIO MOREIRA DOS SANTOS, Neutron Sciences Directorate, ORNL, Oak Ridge, TN, USA, KUO LI, Geophysical Laboratory, Washington, DC, USA, JAMIE MOLAIISON, Neutron Sciences Directorate, ORNL, Oak Ridge, TN, USA, RUSSELL HEMLEY, Geophysical Laboratory, Washington, DC, USA — The symmetrisation of the H-bonds in water was first predicted almost 60 years ago [1]. In subsequent decades, the formation of symmetric ice X has been extensively studied. Neutron-diffraction studies of \( \text{D}_2\text{O} \) ice [2,3] are particularly useful in characterising the structure, providing the only direct measurements of the proton (deuteron) density distribution. However, to date, a limited maximum pressure (of <30 GPa) for these studies has confined them to a regime where the water molecule geometry remains essentially unchanged from ambient pressure [3]. We will present an implementation of diamond-anvil-cell techniques for neutron powder diffraction at the SNS, Oak Ridge TN. This new capability permits neutron structural measurements up to at least 70 GPa. We will show data on crystalline \( \text{D}_2\text{O} \) up to these pressures, which approach those of the symmetrisation transition.

[1] B. Kamb & B.L. Davis PNAS 52 1433 (1964);