Monday, June 25, 2007 8:00AM - 8:30AM — Session A1 Plenary Session I followed by Memorial Session Fairmont Orchid Hotel Salon I/II

8:00AM A1.00001 Applications of Shock Wave Research to Developments of Therapeutic Devices. KAZUYOSHI TAKAYAMA, Tohoku University Biomedical Engineering Research Organization — Underwater shock wave research applied to medicine started in 1980 by exploding micro lead azide pellets in water. Collaboration with urologists in the School of Medicine, Tohoku University at the same time was directed to disintegration of kidney stones by controlling shock waves. We initially proposed a miniature truncated ellipsoidal cavity for generating high-pressures enough to disintegrate the stone but gave up the idea, when encountering the Dornier Systems’ invention of an extracorporeal shock wave lithotripter (ESWL). Then we confirmed its effectiveness by using 10 mg silver azide pellets and constructed our own lithotripter, which was officially approved for a clinical use in 1987. Tissue damage during ESWL was attributable to bubble collapse and we convinced it could be done in a controlled fashion. In 1996, we used 160 ml pulsed Ho:YAG laser beam focusing inside a catheter for shock generation and applied it to the recanalization of cerebral embolism, which is recently expanded to the treatment of pulmonary infarction. Micro water jets discharged in air were so effective to dissect soft tissues preserving small blood vessels. Animal experiments are successfully performed with high frequency water jets driven by an actuator-assisted micro-pump. A metal foil is deformed at high speed by a Q-switched Nd:YAG laser beam loading. We used this technique to project micro-particles or dry drugs attached on its reverse side and extended it to a laser ablation assisted dry drug delivery or DNA introductory system.

Monday, June 25, 2007 10:30AM - 12:30PM — Session B2 Inelastic Deformation-Glass and Porous Media Fairmont Orchid Hotel Amphitheater

10:30AM B2.00001 Dynamic Compaction of Sand1. JUSTIN BROWN, TRACY VOGLER, LALIT CHHABILDA, Sandia National Laboratories — Dynamic compaction of sand was investigated experimentally to stress states of approximately 2 GPa using a special target fixture for accurately measuring shock velocity in porous materials. Experiments were performed in the partial to nearly full compaction region. The Hugoniot state of the sand was determined using the measured velocity interferometer profiles and impedance matching techniques. The velocity interferometer probes located on the rear surface of a stepped target provide accurate measurements of shock velocity by correlating time difference for the four measurements. These results were used to fit parameters for the P-Alpha and P-Lambda models for porous materials for simulating the experiments with the CTH hydrocode.

1 Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000

10:45AM B2.00002 Shock-Loading of Statistically Compacted Sand. DAVID CHAPMAN, CHRISTOPHER BRAITHWAITE, WILLIAM PROUD, University of Cambridge, UK — Herrmann’s P-alpha model has recently been applied the behaviour of porous geological systems. The equation of state is broken into two distinct regions; un-compacted and a fully compacted. In an effort to improve understanding of the compaction process plate-impact experiments have been conducted on compacted sand. Sand is quasi-statically compacted prior to shock loading. The Hugoniot curve for the densified material is obtained and compared with that of the uncompacted material.

11:00AM B2.00003 The Dynamic Compaction of Sand and Related Porous Systems, WILLIAM PROUD, Cavendish Laboratory, University of Cambridge — Porous and granular materials are widely found in a number of environments. One of the most important groups both geographically and in the construction industry are the sands. A review of the response of sand (42% porous) and a very low-density silica dust (95% porous) will be presented as well as recent data. Strain rates will be from quasi-static to the shock regime, effects such as grain size, humidity, will be discussed.

In collaboration with David Chapman and Kostas Tsembeis, Cavendish Laboratory, University of Cambridge; Philip Church and Ian Cullis, QinetiQ, Fort Halstead, UK; David Porter, Fanborough, UK; Peter Gould, QinetiQ, Bristol; Anatoly Bragov and Andrey Lomunov, University of Nizhny Novgorod, Russia; John Borg, Marquette University, Wisconsin, USA; and John Cogar, Corvid Technology, USA.

11:30AM B2.00004 On the shock response of soda lime glass, ZVI ROSENBERG, RAFAEL, NEIL BOURNE, University of Manchester — The response of brittle materials to shock has attracted attention for the past thirty years. Yet there are still unexplained aspects to the observed behaviour. In particular it is agreed that a failure front propagates behind the shock, travelling at an approximately constant velocity. Over the past years we have used embedded sensors, remote imaging and surface velocity measurement to track these phenomena. In the present paper, lateral measurements of strain are used to track three dimensional flow occurring behind the failure front. This is related to observations of the various thresholds observed in behaviour commented upon previously. A review of the behaviour of soda lime glass under impact is presented to unify these data.

11:45AM B2.00005 A study of pre-stress effect on the failure waves in glasses, ANDREY SAVINYKH, Institute of Problems of Chemical Physics, GENNADY KANEL, Joint Institute for High Temperatures, SERGEY RAZORENOV, Institute of Problems of Chemical Physics, A. RAJENDRAN, U.S. Army Research Office — Results of shock-wave experiments with free and pre-stressed samples of K8 crown glass, K14 crown glass and fused quartz are presently in Controlled confinement pressure on the specimen in the range of 200 MPa to 300 MPa was provided by installing a shrink-fit metal sleeve on the lateral surface of the sample disk. The shock compression pulses of approximately triangular profile were created using thin aluminum impactors and PMMA base plates. The peak shock pressures in the range of 5.5 GPa to 8.5 GPa were sufficient to initiate the failure waves, whereas following unloading stopped the cracking. Results of measurements of the free surface velocity histories show that pre-stressing results in earlier braking of the failure wave. Thus, the compressive transversal stress increases the failure threshold that is in agreement with existing criteria of compressive fracture. The work was supported by the US Army Research Office through CRDF GAP grant number RUE2-1615-MO-06.

12:00PM B2.00006 Dynamic Response of Soda-Lime Glass1. C. SCOTT ALEXANDER, Sandia National Laboratories — Soda-lime glass (SLG) is a highly available low cost glass formulation commonly used in window applications and it may have potential use in transparent ceramic armor. While there has been a great deal of work done to characterize the shock response of fused silica, the primary component of SLG, comparatively little is known about SLG itself. This paper will report the results of characterization experiments conducted at Sandia National Laboratories on a low iron content soda-lime glass commercially available from PPG Industries. Data have been collected over a wide range of stress levels from 4 to 65 GPa. Topics will include the Hugoniot response including non-linear elastic behavior, support for a high stress phase transition, material strength, and evidence for failure of the material under certain conditions. Further, the results will be compared and contrasted with related findings in fused silica as well as work on similar soda-lime glass formulations reported by other researchers.

1 Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
10:30AM B3.00001 Radical electronic transformation of strongly coupled plasma at megabar pressure ionization, dielectrization and phase transitions, VLADIMIR FORTOV, IHED RAS — The work presents new results of investigation of pressure and temperature ionization of coupled nonideal plasmas generated as a result of multiple shock compression of metals, H2, He, noble gases I, fullerene C60, H2O in the megabar pressure range. The highly time-resolved diagnostics in the ultrafast (ns to fsec), radiative and mechanical properties of high pressure condensed matter in a broad region of the phase diagram. This data in combination with exploding wire conductivity measurements demonstrate an ionization rate increase up to ten orders of magnitude as a result of compression of degenerate plasmas at p 104-107 bars. Shock compression of H2, Ar, He, Kr, Ne, Xe in initially gaseous and cryogenic liquid state allows measuring the electrical conductivity, Hall effect parameters, equation of state, and emission spectra of strongly nonideal plasma. Thermal and pressure ionization of strongly coupled states of matter is the most prominent effects under the experimental conditions. It was shown that plasma compression strongly deforms the ionization potentials, emission spectra and scattering cross-sections of the neutrals and in the strongly coupled plasmas. In contrast to the plasma compression the multiple shock compression of solid Li, Na, Ca shows “dielectrization” of the elements. Phase transitions in strongly nonideal plasmas are discussed.

10:45AM B3.00002 The Equation of State and Optical Conductivity of Warm Dense He and H2, STEPHANIE BRYGOO, JON H. EGGERT, LLNL, PAUL LOUBEBYE, CEA, RYAN S. MCMILLIANS, UC Berkeley, DAMIEN G. HICKS, PETER M. CELLIERS, LLNL, TOM R. BOEHL, LLE, RAYMOND JEANLOZ, UC Berkeley, GILBERT W. COLLINS, LLNL — The determiniation of the equations of state of helium and hydrogen at very high density is an important problem at the frontier between condensed matter physics and plasma physics with important implications for planetary physics. Due to the limitations of the conventional techniques for reaching extreme densities (static or single shock compression), there are almost no data for the deep interior states of Jupiter. We present here shock compression measurements of helium and hydrogen, precompressed in diamond anvil cells up to 3.5 GPa. We report the shock pressure, density and reactivity up to 2 Mbar for helium and up to 1 Mbar for hydrogen. The data are compared to equations of state models used for astrophysical applications and to recent first principles calculations. This work was performed under the auspices of the U.S. Department of Energy (DOE) by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

11:00AM B3.00003 Simulations of Shocked Hydrogen and Helium and Implications for Giant Planet Interiors, BURKHARD MILITZER, Carnegie Institution of Washington — In 1996 the NOVA laser shock wave experiments at LLNL probed the properties of deuterium at megabar pressure for the first time. These measurements have triggered a large number of theoretical and experimental studies. Recently the combination of static and dynamic compression techniques allowed one to reach even higher densities. In this talk, path integral Monte Carlo and density functional molecular dynamics simulations have been applied to predict the shock states of precompressed hydrogen and helium samples. It will be explained why the precompression leads to a reduction in the compression ratio for both materials [1]. It will also be demonstrated that electronic excitations lead to a much higher compression ratio of 5.24 for shocked helium compared to 4.3 that our simulations predicted for deuterium. Combining our equation of state (EOS) results for shock samples with further first-principles simulation for hydrogen-helium mixtures [2] allowed us to build a model for the interiors of giant planets. Included were corrections to the commonly used linear mixing approximation as well as the increased stability of hydrogen molecules that arises from the presence of helium. Our interior models update the suite of models that were based on the widely used Saumon-Chabrier-Van Horn (SCVH) EOS. Deviations from SCVH are up to about 5 percent depending on the pressure, and thus affect interior models at the same level. Unlike SCVH, the computed DFT-EOS does not predict any first-order thermodynamic discontinuities associated with pressure-dissociation and metatllization of hydrogen [2]. We conclude by discussing constraints for the size of Jupiter’s rocky core and whether the planet was formed by core accretion.


11:30AM B3.00004 Equation of state measurements in Ta2O5 aerogel, JOSHUA MILLER, TOM BOEHLY, DAVID MEYERHOFER, University of Rochester, JON EGGERT, Lawrence Livermore National Laboratory — The examination of the equation of state of Ta2O5 aerogel using laser driven shock compression has been performed at OMEGA. The foams, with densities in the range of 0.1 to 0.25 g/cc, were loaded by shocks with pressures in the range of 50 to 300 GPa. Hugoniot parameters inferred from mechanical measurements of the shock evolution and temperatures inferred from the shock front self-emission were resolved on the sub-nano-second time scale during this study. Comparisons between these experimental results and the existing qEOS model show that the aerogel is much more compressible than qEOS predicts at pressures below 100 GPa. This work was supported by the U.S. Department of Energy Office of Inertial Confinement Fusion under Cooperative Agreement No. DE-FC03-92SF19460, the University of Rochester, and the New York State Energy Research and Development Authority. The support of DOE does not constitute an endorsement by DOE of the views expressed in this article.

11:45AM B3.00005 Multi-Megabar pressure and super-dense materials created by induced micro-explosion inside of transparent solid, EUGENE GAMALY, Australian National University, Canberra, Australia, SAULIUS Joudkazis, HIROAKI MISAWA, Hokkaido University, Sapporo, Japan, BARRY LUTHER-DAVIES, ANDREI RODE, Australian National University, Canberra, Australia, LUDOVIC HALLO, PHILIPPE NICOLAI, VLADIMIR TIKHONCHUK, Universite Bordeaux1, France — High pressure and temperature have been achieved using a single laser pulse (100 nJ, 800 nm, 200 fs) focused inside transparent dieslectrics [1,2]. The laser pulse converts a material within the volume of the laser focal spot into plasma. The plasma is then compressed by the hydrodynamic compression of the shell of compressed material. Analysis of the size of the void and the shell as a function of laser energy revealed that shell has a density 1.14 times of sapphire. We report here the pressure and reflectivity up to 2 Mbar for helium and up to 1 Mbar for hydrogen. The data are compared to equations of state models used for astrophysical applications and to recent first principles calculations. This work was performed under the auspices of the U.S. Department of Energy (DOE) by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

2:00PM B3.00006 Charged particle flows in an explosively generated non-ideal plasma, C.J. BOSWELL, J.R. CARNEY, J. WILKINSON, G.I. PANGILINAN, Indian Head Division, NSWC, V.H. WHITLEY, LANL — Non-ideal plasmas occur as a result of the stimulation of matter by strong shocks, detonation waves, or concentrated laser irradiation. Since all of these methods of generating non-ideal plasmas are already in use to address other problems, we focus on a detailed understanding of this plasma. In particular, we study the flow of charged particles in a non-ideal plasma generated using an explosive to compress the gas into the non-ideal plasma state. The shock wave in the gas is generated by an explosive located at one end of a guide tube filled with the gas. The detonation produces a shock wave strong enough to ionize the gas. Spectral line emission profiles, recorded with a streak emission spectroscopy system, are used to ascertain neutral and ionized gas properties. The electric and magnetic fields are measured by electrostatic probes and magnetic induction coils which permit the measurement of the temperature, density, and electric potential of the non-ideal plasma, as well as the flow of net electric charges respectively. The results demonstrate that a separation of the positive and negative charges occurs in the vicinity of the shock wave.

Monday, June 25, 2007 10:30AM - 12:30PM
Session B3 High Energy Density Physics / Warm Dense Matter
Fairmont Orchid Hotel Plaza I
of state and phase transitions under various controlled loading and a two-dimensional displacement interferometer were utilized for time-resolved measurements. Some targets and substrates were recovered and examined. Gaussian, ramping, and Taylor-release pulses (the latter two were the first and second half of a full Gaussian pulse, respectively). The point- and line-VISAR materials examined included Cu, Be and Ta. The laser pulse durations ranged from about 100 ns to 2 ns (wavelength of 1054 nm), and its shapes, from Gaussian, ramping, and Taylor-release pulses (the latter two were the first and second half of a full Gaussian pulse, respectively). The point- and line-VISARs and a two-dimensional displacement interferometer were utilized for time-resolved measurements. Some targets and substrates were recovered and examined. We have also devised a new technique to measure M-band radiation preheat. These hohlraums will be extended to NIF in 2008. (1) R.F. Smith, S.M. Pollaine, S.J. Moon, H.S. Park, K.T. Lorenz, P.M. Celliers, J.H. Eggert, G.W. Collins, “High planarity x-ray drive for ultra-fast shockless-compression experiments,” accepted Physics of Plasmas (2007)

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

Monday, June 25, 2007 10:30AM - 12:30PM –
Session B4 Experimental Developments I Fairmont Orchid Hotel Plaza II

10:30AM B4.00001 Coherent THz frequency radiation from shock waves: A new ultrafast strain wave detection mechanism1, EVAN REED, MICHAEL ARMSTRONG, Lawrence Livermore National Laboratory, KYIYONG KIM, JAMES GLOWNIA, Los Alamos National Laboratory — Using molecular dynamics simulations and analytics, we predict that large amplitude strain and shock waves can generate detectable electromagnetic radiation at an interface between two different piezoelectric materials. This new form of radiation generation is coherently related to the temporal profile of the strain wave propagating past the interface and can be utilized as a wireless ultrafast strain wave detector with potentially unprecedented subpicosecond time resolution. We present the first experimental observation of this effect at an interface between aluminum and GaN and find excellent agreement with picosecond timescale simulations.

1This work was performed under the auspices of the US Department of Energy by the University of California, LLNL under contract number W-7405-Eng-48.

10:45AM B4.00002 Development of third harmonic generation as a short pulse probe of shock heated material, WILL GRIGSBY, MICHAEL DOWNER, The University of Texas at Austin, JEFF COLVIN, Lawrence Livermore National Laboratory, TODD DITMIRE, The University of Texas at Austin — We are studying laser-produced shock waves in silicon (100) at pressures up to 1.5 Mbar. To examine the material dynamics, including shock induced melt, we are performing pump-probe experiments utilizing 500 ps and 40 fs laser pulses from a Ti:sapphire laser. Two-dimensional time-resolved interferometry reveals information about the shock breakout, while third harmonic light generated at the rear surface is used to infer the crystalline state of the material as a function of time.

11:00AM B4.00003 Transient Imaging Displacement Interferometry Applied to Shock Loading, SCOTT GREENFIELD, SHENGNIAN LUO, DENNIS PAISLEY, ERIC LOOMIS, DAMIAN SWIFT, AARON KOSKELO, Los Alamos National Laboratory — We have applied Transient Imaging Displacement Interferometry (TIDI) to copper and beryllium samples subjected to various loading methods. TIDI captures the full-field out-of-plane surface displacement map single-shot with the time resolution of the illumination pulses (ca. 100 ps). Displacement sensitivity of better than 10 nm with laterally spatial resolution of roughly 5 microns is achieved over our ca. 1 mm2 field-of-view. A framing camera allows capture of up to eight displacement maps for a single loading event, allowing the evolution of the surface motion to be tracked. Loading methods using the TRIDENT laser at Los Alamos have included laser-launched flyers, direct drive, and confined ablation. Point and line VISARs are used as complementary diagnostics that provide a temporally continuous record of the velocity history of the sample, and also provide time stamps for the TIDI displacement maps. The rich heterogeneity in the surface displacement due to the grain structure of the sample is readily measured. We will use TIDI to attempt to observe small voids in the regime of incipient spall, and track the dynamics of their growth. Other experiments will quantify shock roughening on ICF-related targets.

11:15AM B4.00004 Study of Underwater Shock Compaction Device for Compaction of Titanium Diboride Powder, G.B. KENNEDY, Y.K. KIM, K. HOKAMOTO, S. ITOH, Kumamoto University — Shock compaction for powders has been used to study bulk consolidation of powder materials. Shock compaction has the advantage of processing at low temperatures and short duration to limit effects of high temperatures for long times, such as increased grain size and high energy cost. Many methods of shock loading of powders have been employed: direct contact with explosive, explosively driven flyer plates, and flyer plates launched with light gas or propellant gun. Another method, using explosives to create a shockwave in water that is in contact with a powder container, has been used extensively at Kumamoto University. This work presents a study of the development of the underwater shockwave device and investigates the water container geometry for control of parameters for shockwave peak pressure, duration, and distribution through the powder compaction process. Results of simulations for optimization of shock compaction properties are presented along with measurements from input and propagated manganin gauge pressure measurements obtained from underwater shock compaction of titanium diboride. The hardness measurements throughout the bulk of the shock compacted titanium diboride are discussed.

11:30AM B4.00005 Dynamic loading with confined laser ablation: An experimental study, SHENG-NIAN LUO, DENNIS PAISLEY, ERIC LOOMIS, SCOTT GREENFIELD, RANDALL JOHNSON, Los Alamos National Lab — We investigated dynamic response of solids with the confined laser ablation technique. A disk-shaped specimen was sandwiched between and in tight contact with a window material and a transparent substrate: an absorbing coating (e.g., Al or graphite) was applied to the substrate surface in contact with the sample in most cases. The materials examined included Cu, Be and Ta. The laser pulse durations ranged from about 100 ns to 2 ps (wavelength of 1054 nm), and its shapes, from Gaussian, ramping, and Taylor-release pulses (the latter two were the first and second half of a full Gaussian pulse, respectively). The point- and line-VISARs and a two-dimensional displacement interferometer were utilized for time-resolved measurements. Some targets and substrates were recovered and examined. Our experiments demonstrate the potential of the confined laser ablation technique for investigating the mechanical properties (plasticity and spall), equation of state and phase transitions under various controlled loading—unloading histories.
11:45AM B4.00006 Experimental Method for Laser-driven Flyer Plates for 1-D Shocks using the TRIDENT Laser1. DENNIS PAISLEY, SHENGNIAN LUO, DAMIAN SWIFT, SCOTT GREENFIELD, ERIC LOOMIS, RANDALL JOHNSON, PEDRO PERALTA, Los Alamos National Laboratory, LDRD TEAM — One-dimensional shocks can be generated using flyer plates accelerated to terminal velocities by a confined laser-ablated plasma. Over the past few years, we have developed this capability with our facility-size laser, TRIDENT, capable of > 500 Joules at multi-microsecond pulse lengths to accelerate 1-D flyer plates, 8-mm diameter by 0.1 – 2 mm thick. Plates have been accelerated to terminal velocities of 100 to >500 m/s, with full recovery of the flyer and target for post mortem metallography. By properly tailoring the laser temporal and spatial profile, the expanding confined plasma accelerates the plate away from the transparent sapphire substrate, and decouples the laser parameters from shock pressure profile resulting from the plate impact on a target. Since the flyer plate is in free flight on impact with the target, minimal collateral damage occurs to either. The experimental method to launch these plates to terminal velocity, ancillary diagnostics, models, and representative experimental data will be presented. LA-UR-07-1111

1 Operated by Los Alamos National Security LLC for DOE/NNSA

12:00PM B4.00007 A Compact Pulser for Magnetically Driven Isentropic-Compression Experiments1, R.B. SPIELMAN, Ktech Corporation, M. BAVAY, J.A. MERVINI, Ivanhoe Technologies Inc., G. AVRILLAUD, ITHPP — The use of magnetic fields to isentropically compress materials for equation-of-state studies has been demonstrated on Sandia National Laboratories’ Z machine. Sharing similarities with the GEPI pulser at the Centre de Etudes de Gramat in France, a compact pulser has been designed and built specifically for isentropic compression experiments. In order to be compact and low cost, the design uses a solid dielectric transmission line to couple current from eight low-inductance Haefely capacitors that are switched with ultra-low-inductance multi-channel gas switches. A peaking stage made of 72 General Atomics capacitors enhanced by a low-inductance, multi-channel peaking switch brings the fundamental rise time of the pulser down to 350 ns (10-90%). A variable inductance in parallel with the peaking switch as well as using various gases in the switch allow us to control the details of the current wave shape. The pulser delivers a peak current of 4 MA at a charge voltage of 80 kV into a short circuit. The rise time can be lengthened to greater than 650 ns to deliver a current of 4.2 MA. The performance of this pulser will be described along with potential design changes that would provide decreases in current rise time and increases in current delivered to real world loads.

12:15PM B4.00008 ABSTRACT WITHDRAWN

Monday, June 25, 2007 10:30AM - 12:30PM — Session B5 Spectroscopy and Optical Studies I Fairmont Orchid Hotel Plaza III

10:30AM B5.00001 Optical Response of Molecular Crystals to Non-hydrostatic Compression in a Diamond Anvil Cell Experiments1, ZBIGNIEW A. DREGER, Washington State University — High pressure response of molecular crystals is not as well understood as the response of covalent or ionic crystals. Because molecular crystals are highly compressible, small variations in applied stresses result in large intermolecular changes. Additionally, low symmetries, characteristic of molecular crystals, result in significant deformation under static pressure loading. Hence, an understanding and controlling of non-hydrostatic effects are important for examining molecular crystals. Several examples will be presented to show the significance of non-hydrostaticity on the underlying molecular mechanisms in a diamond anvil cell experiments. In particular, we will present our work on selected molecular crystals to highlight the role of non-hydrostaticity on: (i) structural phase transitions, (ii) changes in electronic structure, (iii) formation of structural defects, and (iv) solid state reactivity. Finally, we will demonstrate a relevance of non-hydrostatic compression to shock wave experiments. Work supported by DOE and ONR.

1 Collaboration with Y. M. Gupta is acknowledged

11:00AM B5.00002 Brillouin-scattering Determination of the Acoustic Properties of Polymers at High Pressure, DANA DATTELBAUM, LEWIS STEVENS, EDWARD ORLER, Los Alamos National Laboratory, Los Alamos, NM 87545, MUHTAR AHART, RUSSELL HEMLEY, Geophysical Laboratory, Carnegie Institute of Washington, 5251 Broad Branch Road NW, Washington, D.C. 20015 — Brillouin scattering is a powerful tool for probing the elastic properties of materials. Coupled with high pressure environments, such as those accessible using diamond anvil cells, the method can reveal rich materials physics under extreme conditions, and provide fundamental data for the development of equations-of-state. For the first time, the acoustic properties of three polymeric elastomers have been measured from ambient pressure to 12 GPa. While both transverse and longitudinal modes were observed for all three polymers, transverse modes were only observed at elevated pressures, with the pressure on-set of observable modes differing for the polymers studied. From the measured acoustic properties, elastic constants, moduli, and Poisson’s ratios were calculated as a function of pressure. P-V isotherms were also constructed, and fit to a range of empirical/semi-empirical isothermal equation-of-state (EOS) forms. From this analysis, the isostructural bulk modulus and its pressure derivative were obtained for the polymers interrogated, and the static results were compared to available shock wave compression data.

11:15AM B5.00003 Time-resolved emission spectroscopy of transparent and nontransparent materials, TAKAMICHI KOBAYASHI, TOSHIMORI SEKINE, National Institute for Materials Science — Time-resolved emission spectroscopy with pulsed excitation has been used to observe spectral changes of shocked transparent single crystals and nontransparent materials. For transparent single crystals, drastic spectral changes near the HEL are observed and Us-Up relations can be determined. As the shock pressure is increased in the plastic region, however, the emission intensity decreases rapidly, probably because plastic deformation develops with pressure. For nontransparent materials, measurements of emission spectra under shock compression appears more difficult than transparent materials. Results on powder materials will be presented.

11:30AM B5.00004 Photoacoustic Measurements to Determine Acoustic Velocities in Shocked Liquids, N. HEMMI, K. ZIMMERMAN, J.M. WINEY, Y.M. GUPTA, Wash. State Univ., D.H. TORCHINSKY, K.A. NELSON, MIT — Experimental developments were carried out to implement the Impulsively Stimulated Thermal Scattering (ISTS) method in shock wave experiments. This method, an application of Brillouin scattering in the time domain, allows us to determine the sound velocity and acoustic damping properties under dynamic loading in single event experiments. We discuss our experimental developments where the capability for performing reproducible single-shot experiments is key. We also present experimental results for benzene and glycerol, highlighting the differences in the shock response for these two liquids. Sound velocities were clearly observed for benzene shocked up to 0.85 GPa, while ISTS signals from shocked glycerol could not be observed due to strong acoustic damping. Implications of these photoacoustic measurements for understanding the shocked state will be presented. Work supported by DOE and ONR.
11:45AM B5.00005 A shock pressure induced phase transition from liquid to solid of cyclohexane using time-resolved coherent anti-Stokes Raman spectroscopy. SHIRO OGUCHI, AKIRA SATO, KEN-ICHI KONDO, KAZUTAKA NAKAMURA — The liquid-solid phase transition of cyclohexane has been studied under laser shock compression up to 3.8 GPa by using nanosecond time-resolved Coherent Anti-stokes Raman Spectroscopy (CARS) and laser shock compression. The shock wave is generated by irradiation of 10 ns pulse laser beam on the plasma confinement target and its pressure is estimated from a particle velocity, which is measured by optically recording velocity interferometer system (ORVIS). Higher frequency shift of the Raman peaks (ring-breathing, C-C stretching, and CH₂ twist modes) was observed at high pressure. At 3.8 GPa, splitting of the peak (CH₂ twist mode) due to change in symmetry of surrounding molecules, which corresponds to phase transition to solid IV, was observed at delay time of 20 ns. Rapid liquid-solid phase transition has been directly observed to occur within 20 ns.

12:00PM B5.00006 Ultrafast shock wave coherent dissociation and spectroscopy of materials. DAFA DLOTT, ZHAOUII WANG, ALEXEI LAGUTCHEV, JEFFREY CARTER, DAVID CAHILL, University of Illinois at Urbana-Champaign — This research is focused on understanding what happens at the level of individual molecules, when a solid is broken into two pieces creating a nascent interface. Ordinarily, breaking a material involves nucleation or crack formation, so that at a given instant every atom at the interface acts differently. In order to get at detailed mechanisms it is desirable to have every atom doing exactly the same thing, in other words to cause the material to dissociate coherently. In this talk we will discuss methods for creating coherence in the dissociation process using femtosecond laser-driven tensile shocks, and methods for probing the molecular structures and energy dissipation processes in atomic layers immediately adjacent to the interface, using nonlinear and coherent optical spectroscopies. This material is based upon work supported by the U.S. Department of Energy, Division of Materials Sciences under Award No. DEFG02-91ER45439, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign.

12:15PM B5.00007 Optical Properties, Raman Scattering, and Radiometry of Diamond under Shock Compression. R. STEWART MCMILLIANS, DYLAN K. SPAULDING, RAYMOND JEANLOZ, University of California Berkeley, JON H. EGEBERT, PETER M. CELLERS, DAMIEN G. HICKS, GILBERT W. COLINS, Lawrence Livermore National Laboratory — We have studied the optical transparency, luminescence, index of refraction, and elastic-plastic relaxation of diamond shocked to pressures in excess of its elastic limit. Techniques include VISAR velocimetry, optical pyrometry, and spontaneous Raman scattering on quasi-steady shock compressions in crystallographic orientations (100), (110), and (111) driven by the kilojoule Janus laser at Lawrence Livermore National Laboratory. We extend the pressures to which diamond, or any material, has been studied using Raman scattering, and explore the development of two-wave, elastic-plastic compression near the Hugoniot Elastic Limit. This work was performed under the auspices of the U.S. Department of Energy, by Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

Monday, June 25, 2007 10:30AM - 12:30PM
Session B6 Detonation Properties Fairmont Orchid Hotel Promenade I/II

10:30AM B6.00001 Microenergetics: Combustion and Detonation at Sub-Millimeter Scales¹. ALEXANDER S. TAPPAN, 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.¹ Our approach is to apply technologies developed by the microelectronics industry to fabricate test samples with well-defined geometries. Substrates have been fabricated from materials such as silicon and ceramics, with channels to contain the energetic material. Energetic materials have been loaded into the channels, either as powders, femtosecond laser-micromachined pellets, or as vapor-deposited films. Ignition of the samples has been achieved by simple hotwires, integrated semiconductor bridges, and also by lasers. Additionally, grain-scale patterning has been performed on explosive films using both oxygen plasma etching and femtosecond laser micromachining.² We have demonstrated simple work functions in microenergetic devices, such as piston motion,¹ which is also a relevant diagnostic to examine combustion properties. Detonation has been achieved in deposited explosive films, recorded by high-speed photography.³ A review of progress on manufacturing and testing will be presented, as well as historical perspectives and future directions.

¹A. S. Tappan, et al., 12th International Detonation Symposium (San Diego, CA, 2002).
²A. S. Tappan, et al., 36th International Annual Conference of ICT, combined with 32nd International Pyrotechnics Seminar (Karlsruhe Federal Republic of Germany, 2005).

11:00AM B6.00002 Micro-Gap Experiments and Insensitive Explosives, RALPH MENIKOFF, LANL — Early research on shock desensitized plastic-bonded explosives (circa 1970) also studied large single crystals of explosive. High quality crystals — free from voids that serve as nucleation sites for hot spots — have been found to be very insensitive to shock initiation. In fact, experiments were not able to initiate a large single crystal of HMX (~ 10 mm) with a detonation wave in PBX 9404, which is 94 weight % HMX and has a Chapman-Jouguet pressure of 35 GPa. Yet a single crystal of HMX can be initiated by a flyer plate that drives a shock at a similar pressure. This is especially puzzling since the detonation wave in PBX 9404 has a peak pressure at the von Neumann spike of nearly 60 GPa. An important difference between the two drive systems is a small gap at the PBX 9404/HMX interface due to surface roughness of the PBX; estimated to be 30 to 50 microns. Conceptually, the experiment is equivalent to the gap test used to compare the sensitivity of different explosives; albeit with a micro-gap and a very insensitive explosive. The inability of a PBX 9404 detonation wave to initiate a single crystal of HMX is due to the reaction zone in the PBX 9404 being of comparable length to the gap in the experiment and the rarefaction or Taylor wave behind the detonation wave.

11:15AM B6.00003 The Incidental Effects of Gaps in Detonating PBX 9501¹. TERRY SALYER, LARRY HILL, Los Alamos National Laboratory — The incidental effects of gaps in detonating explosives have been observed for many years, yet the root cause of peripheral damage due to these features has been a partial mystery. To evaluate such damage for PBX 9501, a test series has been performed that examines single and multiply-directed detonations both crossing and moving along gaps of varying widths, lengths, and angles relative to the detonation wave fronts. Damage is evaluated with steel witness plates and quantified through trench profiling, volume, and mass decrement measurements. In addition, streak camera traces are used to track detonation wave speeds along explosive material surfaces and across gaps. Such traces allow the quantification of timing delays due to gap reinitiation processes for both confined and unconfined explosives. For some reinitiation tests, a second detonation wave is directed to interfere at varying times with the post-gap run-up process of the first wave, thus allowing complex wave-wave interactions to be investigated in detail. With these cumulative observations, further insight into the mechanism of extrinsic damage due to gaps is gained.

¹Work supported by the United States Department of Energy.
corner turning situations. But there the detonation borders with a dead zone, and the boundary contour is not known in advance. This finite rise time effect near a low impedance boundary plays a role also in calculations of reactive flow calculations of detonation in a rod, an unreacted layer is formed at the boundary, affecting the diameter effect outcome. We investigate the origin of one-dimensional experimental data.

that is able to reproduce a range of shock initiation behaviour in conventional plastic bonded explosives. This is accomplished by using entropy rather than reaction rates to model shock initiation and detonation behaviour in plastic bonded explosives. To date the model has been applied to a wide range of shock initiation data obtained from explosive gas-gun experiments where one-dimensional, planar, flat-topped shocks are delivered to the explosive samples. In this paper, to provide a more rigorous test of CREST’s predictive capability, the model is applied to two-dimensional explosive experiments where the shock wave entering the explosive departs from the ideal gas-gun case. The calculated results show that the model can simulate the explosive response in shock regimes that are markedly different from truly one-dimensional conditions. This gives confidence in the ability of CREST to simulate a wide range of shock initiation and detonation phenomena.

Measured peak pressure is approximately 600 times greater than that in a divergent front resulting from point initiation.

Reaction rates to model shock initiation and detonation behaviour in plastic bonded explosives. To date the model has been applied to a wide range of shock initiation data obtained from explosive gas-gun experiments where one-dimensional, planar, flat-topped shocks are delivered to the explosive samples. In this paper, to provide a more rigorous test of CREST’s predictive capability, the model is applied to two-dimensional explosive experiments where the shock wave entering the explosive departs from the ideal gas-gun case. The calculated results show that the model can simulate the explosive response in shock regimes that are markedly different from truly one-dimensional conditions. This gives confidence in the ability of CREST to simulate a wide range of shock initiation and detonation phenomena.

11:45AM B6.00005 Supra-Pressure Detonation of Aluminized Explosive, RONALD BROWN, B. KAROSICH, J. GAMBLE, J. STORK, A. BIESTERVELD, T. MOORE, J. SINIBALDI, Naval Postgraduate School, M. WALPOLE, A. LINDFORS, K. JACKSON, R. KOONTZ, D. THOMPSON, NAWC-China Lake — Results suggest that there is a continuum of reactions induced behind a supra-pressure convergent shock front in explosive cores of coaxial charges. The pressures in convergent fronts continually increase at an increasing rate from the circumference to the charge axis. Furthermore the unreacted explosive envelope. In these experiments we find a long lived dead-zone consisting of shocked explosive that persists to very late times. Data and numerical modeling will be presented in addition to a comparison with previous work using an external air well. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

11:15AM B7.00004 Reactive Flow Calculation near a Free Boundary, YEHUDA PARTOM, RAFAEL — In reactive flow calculations of detonation in a rod, an unreacted layer is formed at the boundary, affecting the diameter effect outcome. We investigate the origin of this boundary layer, and propose a simple and practical way to eliminate it. We show that it is an artifact of the finite rise time of the shock, caused by artificial viscosity. When the shock reaches a boundary cell, it releases right away, so that pressure and temperature there only reach a fraction of their shock levels, and the reaction rate is slow. We propose to remedy this artifact by delaying the boundary motion for a short while (40 nsec for a 10 cells per mm mesh) after arrival of the shock. In this way the boundary cells reach the appropriate pressure and temperature and react at the appropriate rate. In the paper we show how this remedy works. We compute detonation in a rod with different values of the boundary motion delay, compare the breakout curve from the far end with data from the literature, and obtain good agreement. This finite rise time effect near a low impedance boundary plays a role also in calculations of corner turning situations. But there the detonation borders with a dead zone, and the boundary contour is not known in advance.
11:30AM B7.00005 A computational study of microstructure effects on shock ignition sensitivity of pressed RDX, YUICHIRO HAMATE, RUTH LU, University of Florida, YASUYUKI HORIE, AFRL/MNME Eglin AFB — There are many experimental measurements of microstructure effects on shock sensitivity and performance of solid explosives. But comparatively speaking, there are very few numerical models of these effects. This paper presents a computational experiment of microstructure effects using a recently developed model (Y. Hamate and Y. Horie, Shock Waves, V. 16, 125 (2006)). The model has been developed aiming at expanding predictive capability and applicability. To increase model capability, it is important to focus on physics-based approach, rather than parameter-fitting approach where non-physical parameter(s) needs to be re-calibrated for different set of conditions. Our model explicitly treats specific surface area with an assumption of exponential size distribution of hot-spots. Experimentally, Khasainov et al. discussed effects of specific surface area and found that both run distance to detonation and critical diameter have linear relation with reciprocal of specific surface area of HE. Computational experiments are carried out using pressed RDX model with various initial specific surface areas that are determined by average explosives particle size. The results demonstrate that both Pop-plots and critical diameter show the linear relation as observed by Khasainov et. al.

11:45AM B7.00006 Physics-Based Reactive Burn Model: Grain size effects and binder effects, XIA LU, YUICHIRO HAMATE, University of Florida, YASUYUKI HORIE, AFRL/MNME — We have been developing a physics-based reactive burn (PBRB) model aiming at expanding predictive capability. The PBRB model was formulated based on the concept of a statistical hot spot cell. In the model, thermomechanics and physicochemical features are explicitly modeled. In this paper, we have extended the statistical hot spot model to explicitly describe the ignition and growth of hot spots. In particular, grain size effects are explicitly delineated through introduction of a size-dependent thickness of the hot-region thickness, a size-dependent energy deposition criterion, and a specific surface area. Besides the linear relationships between the run distance to detonation and critical diameter with the reciprocal specific surface area of HE, as discussed in a parallel paper in this meeting, parametric studies have also shown that the PBRB can predict a non-monotonous variation of shock sensitivity with grain size, as observed by Moulard et al. The purpose of this work is to extend the model to include the effects of explosive binders explicitly. As a first step we investigate the thermomechanical effects of a binder by using direct mesoscale simulations. The results will be used in the extending the PBRB model to include binder thermomechanics explicitly.

12:00PM B7.00007 Multi-scale Statistical Design of High Energy Density Materials, JOSEPH C. FOSTER, D. SCOTT STEWART, University of Illinois, KEITH THOMAS, Los Alamos National Laboratory — High energy density materials (HEDM) find wide ranging application in commercial and defense applications. The engineering design of these materials is represented by a hierarchy of specifications on materials and processes. The specifications range in scale from molecular by specifying polymorphic crystal structure to macroscopic specifying geometry and global density. These specifications are used to control the configuration of the production HEDM component in the system design. A formalism analogous to that used in statistical mechanics is presented to aid in the interpretation of physical variability of the design based on specification. A multi-dimensional design space with restrictions imposed engineering specifications is proposed to construct an ensemble of specific designs represented by the variability allowed in the specifications. Based on a physical interpretation of the specifications and how they might apply to the physical function of the component; the formalism is intended to provide a well posed basis for the interpretation of design/ function relationships and fluctuations in behavior.

Monday, June 25, 2007 1:45PM - 3:15PM — Session C2 First Principles and Molecular Dynamics Calculations I Fairmont Orchid Hotel Amphitheater

1:45PM C2.00001 Anisotropic constitutive relationships in energetic materials: nitromethane, RDX, and TATB, IVAN OLEYNIK, MICHAEL CONROY, University of South Florida, CARTER WHITE, Naval Research Laboratory — We extend our first-principles studies of isotropic equation of states (EOS) of energetic materials to include stress-dependent relationships that describe the anisotropic materials response upon dynamic loading. We will discuss the results of first-principles density functional theory calculations of the energetic materials nitromethane, RDX, and TATB. The behavior of the materials is investigated upon both hydrostatic and uniaxial compressions along different crystallographic directions and compressions resulting in pressures up to 50 GPa. We will examine the equations of state for each material, its structural and electronic properties as a function of compression ratio, and compare with available experimental results. The behavior of shear stresses upon uniaxial compression will be discussed in relationship with the sensitivity properties of these materials.

2:00PM C2.00002 Molecular simulations of Crussard curves of detonation product mixtures at chemical equilibrium: Microscopic calculation of the Chapman-Jouguet state, EMERIC BOURASSEAU, VINCENT DUBOIS, NICOLAS DESBIENS, JEAN-BERNARD MAILLET, CEA-DAM — The simultaneous use of the Reaction Ensemble Monte Carlo (ReMC) method and the Adaptive Erpenbeck EOS (AE-EOS) method allows us to calculate directly the thermodynamical and chemical equilibrium of a mixture on the hugoniot curve. The ReMC method allow to reach chemical equilibrium of detonation products and the AE-EOS method constraints the system to satisfy the Hugoniot relation. Once the Crussard curve of detonation products has been established, CJ state properties may be calculated. An additional NPT simulation is performed at CJ conditions in order to compute derivative thermodynamic quantities like Cp, Cv, Gruneisen gama, sound velocity, and compressibility factor. Several explosives has been studied, of which PETN, nitromethane, tetryanitromethane, and hexanitroethane. In these first simulations, solid carbon is eventually treated using an EOS.

2:15PM C2.00003 Ab Initio Equation of State for β-HMX1, FRANK ZERILLI, Naval Surface Warfare Center, Indian Head, MD, MAJIA KUKLJA, National Science Foundation, Arlington, VA — An ab initio equation of state for the molecular crystal β-octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (β-HMX) has been calculated for temperatures between 0 and 400 K, and for specific volumes from 0.42 to 0.55 cm^3/gm, corresponding to relative volumes from 0.8 to 1.03. The calculated 300 K isotherm agrees well with the experimentally measured pressure-volume relation reported by Gump and Periss (J. Appl. Phys. 97, 053513 (2005)), and by Yoo and Cynn (J. Chem. Phys. 111, 10229 (1999)). The calculated specific heat agrees well with experimental data reported over the range from 300 to 400 K (Hanson-Parr and Parr, J. Energetic Mater. 17, 1-47 (1999)). The main source of error in the calculations is due to the absence of an adequate ab initio treatment of non local van der Waals interactions which are important in molecular crystals. Work is underway to include these interactions.

1Work supported by NSWC Core Research Program and by the Office of Naval Research

2:30PM C2.00004 Anisotropic constitutive relationships in energetic materials: PETN and HMX, MICHAEL CONROY, IVAN OLEYNIK, California Institute of Technology, CARTER WHITE, Naval Research Laboratory — One of the important goals in energetic materials (EM) research is predicting EM properties from first principles based upon underlying atomic structure. Special attention is being focused on obtaining accurate equations of state for several important classes of EMs. In this presentation, we will discuss the results of first-principles density functional theory calculations of the energetic materials PETN and HMX. For each material, we have simulated both hydrostatic compression and uniaxial compression in the crystallographic directions [100], [010], [101], [011], and [111] up to V/Vo = 0.50 (~40-50 GPa). We will examine the equations of state for each material and other structural properties of the unit cell as a function of volume and compare with available experimental results. Also, we will discuss the correlation between calculated shear stresses upon uniaxial compression with experimentally observed anisotropies in sensitivity to shock-induced detonation.
2:45PM C2.00005 First principles calculation of the structure and vibrational modes for RDX crystals under static and shock compression\textsuperscript{1} M.S. MIAO, Z.A. DREGER, J.M. WINEY, Y.M. GUPTA, Inst. for Shock Phys.
Wash State Uni. — The structure and vibrational modes for RDX crystals, under hydrostatic pressures up to 4 GPa and uniaxial strains along [100] and [111] directions, were calculated at the first principles level by use of the VASP program. The PW91 generalized gradient approximated (GGA) exchange and correlation energy functional and ultrasoft pseudopotentials were employed and a cutoff of 550 eV was used for plane wave basis. The calculated volume and lattice constants at ambient pressure are larger than the experimental value. With increasing pressure, both volume and lattice constants agree better with experimental values. Despite the large deformation of the lattice, the geometry of each molecule changes only slightly as a function of pressure or uniaxial strain. For the vibrational modes, the calculated pressure dependencies of the frequencies agree well with experimental results. For example, the C-H stretching modes and lattice modes show large pressure dependences whereas many other modes such as the ONO stretching modes change only slightly with pressure. The comparison between the effects of hydrostatic pressure and uniaxial strain on vibrational modes will also be presented.

\textsuperscript{1}Work supported by DOE and ONR.

3:00PM C2.00006 Calculation of RDX molecular crystal geometry and vibrational frequencies under hydrostatic pressure\textsuperscript{1}, WARREN PERGER, WIL SLOUGH, Michigan Tech University — First-principles calculations of the effects of hydrostatic pressure on RDX are performed using the all-electron CRYSTAL06 program. The lattice constants and optimized internal co-ordinates are simultaneously obtained at ambient pressure and hydrostatic pressure up to 4 GPa. A variety of density functionals and basis sets are used and presented for comparison. The vibrational frequencies as a function of pressure are also calculated and compared with previous gas-phase calculations.

\textsuperscript{1}Supported by a ONR-MURI grant

Monday, June 25, 2007 1:45PM - 3:15PM —
Session C3 X-ray Diffraction/Scattering
Fairmont Orchid Hotel Plaza I

1:45PM C3.00001 X-ray scattering measurements from solid density plasmas\textsuperscript{1}, SIEGFRIED GLENZER, Lawrence Livermore National Laboratory, PAUL NEUMAYER, OTTO LANDEN, NATIONAL IGNITION FACILITY PROGRAMS COLLABORATION — The development of spectrally resolved x-ray scattering for accurate measurements of densities and temperatures in solid-density plasmas has enabled new applications to characterize shock-compressed matter. The first proof-of-principle experiments on the Omega laser facility at the Laboratory for Laser Energetics have employed isochorically heated solid-density beryllium targets. In backscattering geometry, Compton scattering measurements have been shown to provide information on temperature and the ionization state from the spectral broadening and relative intensity of the inelastic scattering spectrum, respectively. In the forward scattering regime, the collective plasmon oscillations have been observed providing the local electron density from the frequency shift of the plasmon peak from the incident probe x-ray energy. These results indicate that the simultaneous application of forward (collective) and backward (non-collective) scattering will allow accurate measurements of the compressibility of warm dense matter. New experimental results important for applications to shock-compressed matter will be discussed.

\textsuperscript{1}This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. Supported by LDRD 05-ERI-003.

2:00PM C3.00002 In-situ probing of lattice response in shock compressed materials using x-ray diffraction\textsuperscript{1}, JAMES HAWRELIAK, LLNL — Diagnostics which can probe the lattice response during shock compression offer insight into many key features of the physical phenomena which govern material response. An in-depth analysis of diffraction images of the alpha to epsilon transition in shock compressed single crystal iron offers insight into the transition mechanism of the lattice due to compression along the 100 principal axes. These single crystal diffraction techniques integrate well with molecular dynamics simulations, and have been shown to offer insight into the atomistics of the shock process.

\textsuperscript{1}In collaboration with Hector Lorenzana, Dan Kalantar, and Bruce Remington Lawrence Livermore National Laboratory; Justin Wark, Andrew Higginbotham, and William Murphy, University of Oxford; Kai Kadau and Timothy German, Los Alamos National Laboratory.

2:30PM C3.00003 Real time x-ray diffraction measurements in shocked solids at the Advanced Photon Source , Y.M. GUPTA, S.J. TURNEAURE, K. PERKINS, K. ZIMMERMAN, Washington State University, C.S. YOO, G.W. COLLINS, Lawrence Livermore National Laboratory, G. SHEN, Carnegie Institute of Washington — The Advanced Photon Source provides a number of benefits (high photon numbers, pulsed time structure, and flexible beam properties) to examine the real time x-ray diffraction response of shocked crystals. However, shock wave experiments at a synchrotron facility pose a number of operational challenges, including the coupling of a shock wave driver to the beam line, and appropriate synchronization/gating of detectors. This talk will describe experimental plans and developments underway to utilize either a monochromatic or white beam for x-ray measurements in shocked solids. A compact launcher to achieve impact velocities of \( \sim 1\text{km/s} \) will be presented. Results of ambient measurements, in preparation for the shock experiments planned this summer, will be presented. Work supported by DOE.

2:45PM C3.00004 Temperature Measurements of Shocked Crystals by Use of Nanosecond X-ray Diffraction , WILLIAM MURPHY, ANDREW HIGGINBothAM, JUSTIN WARK, University of Oxford, UK, NIGEL PARK, AWE, Aldermaston, UK — Over the past few years we have been pioneering the use of sub-nanosecond X-ray diffraction to determine the phase and compression of shocked crystals. It is well known that the deviation of atoms from their ideal lattice sites due to thermal motion reduces the integrated intensity within diffraction peaks - the so-called Debye-Waller effect, and thus it is pertinent to investigate whether line ratios might be sufficiently sensitive to be used as a viable temperature diagnostic. Clearly the matter is not completely straight-forward, as the Debye frequency of a solid also varies under compression. In our initial investigations we have calculated the ratios of intensities of high-order reflections assuming various forms of the Gruneisen parameter, and have also compared these results with those obtained from Molecular Dynamics simulations. We also note that under isentropic compression high order reflections monotonically increase in intensity. Given the photon energies of nanosecond X-ray pulses that can currently be produced, we comment on the experimental feasibility of the technique.
3:00PM C3.00005 Measurement of shock wave density using quantitative x-ray phase contrast imaging, DAMIEN HICKS, JON EGGERT, PETER CELLIERS, HYE-SOOK PARK, SEBASTIEN LE PAPE, PRAVESH PATEL, BRIAN MADDOX, GILBERT COLLINS, Lawrence Livermore National Laboratory, THOMAS BOEHLY, University of Rochester, BENJAMIN BARBREL, Ecole Polytechnique — Determining the density in a shock wave at multi-Mbar pressures using traditional impedance matching methods suffers from the dual problems of increasing uncertainty in the material standard and the increasing precision required to measure shock velocities. We present results from laser-driven shock wave experiments employing a technique designed to achieve direct density measurements of a shock wave. Point projection of a laser-plasma x-ray source is used to produce a phase contrast image snapshot of an expanding shock wave. Using an iterative algorithm to determine the propagation of refracted x-rays at the shock front, the resulting optical depth of the image is tomographically inverted to determine the shock density. By simultaneously measuring the shock velocity using VISAR, absolute equation-of-state points are determined. This technique has been extended to produce phase contrast images of shocks in aluminum using high-energy, short-pulse laser-produced x-rays. This work was performed under the auspices of the US DOE by LLNL under Contract No. W-7405-ENG-48 and by the University of Rochester under Cooperative Agreement No. DE-FG03-92SF19460.

Monday, June 25, 2007 1:45PM - 3:15PM –
Session C4 Phase Transitions I Fairmont Orchid Hotel Plaza II

1:45PM C4.00001 Ab initio studies of electronic and structural transitions in low-Z liquids under extreme conditions, STANIMIR BONEV, Dalhousie University, Halifax, NS, Canada — The liquids of group I elements (H, Li, Na, and K) are studied using first principles theory. It will be shown that they undergo electronic and structural transitions analogous to that observed in their solids, but commencing at much lower pressure in the presence of disorder. These changes result in exotic melting behavior and in molten phases with unusual properties. The theoretical predictions will be compared with experimental data and ways for further experimental verification of the theoretical results will be suggested.

1Work supported by the NSERC of Canada.

1:15PM C4.00002 Phase separation in H2O:N2 mixtures and implications for detonation, LAURENCE FRIED, AMITESH MAITI, Lawrence Livermore National Lab, Richard GEE, Sorin Bastea — A class II atomistic force field with Lennard-Jones 6-9 nonbond interactions is used to investigate equations of state (EOS) for important high explosive detonation products N2 and H2O in the temperature range 700-2500 K and pressure range 0.1-10 GPa. A standard 6th order parameter-mixing scheme is then employed to study a 2:1 (molar) H2O:N2 mixture, to investigate in particular the possibility of phase-separation under detonation conditions. The simulations demonstrate several important results, including: (i) the accuracy of computed EOS for both N2 and H2O over the entire range of temperature and pressure considered; (ii) accurate mixing-demixing phase boundary as compared to experimental data; and (iii) the departure of mixing free energy from that predicted by ideal mixing law. The importance of supercritical phase separation during detonation will be discussed. The work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

2:30PM C4.00003 Shock Crystal Growth of Water in Dynamic-DAC, Choong-Shik Yoo, LLNL, William Evans, Geun-Woo Lee — While diamond anvils cells (DACs) and gas-guns are capable of generating high pressures to 300-400 GPa, the precise and tunable control of de/compression rates has been a formidable challenge to both static and dynamic high-pressure research. Furthermore, the pressure-induced polymerization, amorphization, and diffusion controlled crystal growth occur at an intermediate time scale (micro-to-millisecond) of conventional shock and static experiments, for which no compression technology is readily available for in-situ studies. To address this situation, we have recently developed dynamic-DAC (d-DAC) capable of precise controlling of pressure and compression rates at high static pressures. Coupling with time-resolved synchrotron x-ray, optical microscopy, and laser spectroscopy, d-DAC enables one to measure time-resolved structural evolutions of a sample across melting and other phase transitions. In this paper, following the brief description of dynamic-DAC, we will present our recent observations in d-DAC including shock crystal growth of ice VI dendrites and ice VII metastably grown from the stability field of ice VI.

2:45PM C4.00004 Shock Induced Melting Behavior of Eutectic Systems, Chris Adams, Los Alamos National Laboratory — Under equilibrium conditions, melting in multi-phase alloy systems is accompanied by short-range diffusion at inter-phase boundaries. The degree to which diffusion contributes to shock induced melting in simple eutectic systems is still an open question. While there exists a considerable body of previous work on shock induced melting in single phase systems, there has been much less work performed on multiphase systems. We will present the results of a series of gas-gun recovery experiments performed over a range of shock loading conditions, illustrating our observations of shock induced deformation and melting behavior in cast and thermo-mechanically processed Ag-Cu simple eutectic samples. Assessments of the shock wave profiles, shock states achieved, and sound speeds at pressure will be discussed in conjunction with pre-and post-shot microstructural characterization of thermo-mechanically processed pre-shot and recovered materials.

3:00PM C4.00005 TEM observation of disproportionation of mullite and sillimanite under shock compression, Toshiyuki Atou, Nobuaki Kawai, Kazutaka G. Kakamura, Ken-Ichi Kondo, Materials and Structures Laboratory, Tokyo Institute of Technology, Masae Kikuchi, Kansai-Fukushi Laboratory, Tohoku University, Shun Ito, Kunio Yubuta, Institute for Materials Research, Tohoku University — The aluminum silicates, mullite and sillimanite are fundamental raw minerals for the refractory industry and ceramics. Shock compression curves of these materials indicate phase transitions above about 30 GPa. Large volume decrease accompanied with the phase transitions have been attributed to disproportionation to alumina and silica. However, detailed behavior of the disproportionation has not been well understood yet. Using transmission electron microscopy, we confirmed very fine (less than 10 nm) γ-alumina in mullite specimen shock-loaded to 65 GPa. In sillimanite specimen shock-loaded to 54 GPa, γ-alumina was also observed, but the particle sizes were much larger (10-20 nm) than those in mullite specimen, suggesting that the disproportionation in sillimanite specimen occurred at lower shock pressure than in mullite specimen. Furthermore, characteristic nano texture observed in mullite specimen could not be found in sillimanite specimen, which might be caused by difference in crystal structures between mullite and sillimanite.

Monday, June 25, 2007 1:45PM - 3:45PM –
Session C5 Equation of State I Fairmont Orchid Hotel Plaza III
Dynamic Properties of a Lead-Antimony Alloy

ROBERT HIXSON, MARK BYERS, DARCIE DENNIS-KOLLER, Los Alamos National Laboratory — Several shock compression experiments have been done recently on a Lead-Antimony alloy. Data was collected using two experimental configurations. One configuration consisted of a forward impact experiment with a LiF window, and was designed to yield Hugoniot information, and information on strength in compression. Sound speed in the compressed state is also obtained, although with moderate uncertainty. The second experimental configuration was similar to the first, but with no window. The absence of a window will cause a large release wave to be generated at the back side of the flyer plate, and tension generated. This kind of experiment is intended to explore dynamic strength in tension.

2:00PM C5.00002 Hugoniot measurement of gold in pressure range up to 580 GPa, MANABU YOKOO, Materials and Structural Laboratory, Tokyo Institute of Technology, NOBUAKI KAWAI, KAZUTAKA NAKAMURA, KEN-ICHI KONDO — Hugoniot for Au and Cu have been measured in the shock pressure range 170 - 580 GPa with a two-stage light gas gun. Impactor velocities were measured with accuracy of 0.2 % by the Faraday-type electromagnetic sensors (FES) method. Shock velocities were measured with accuracy of 1 - 3 % with the line reflection method (LRM) using a streak camera and Ar ion laser with a few nanosecond time resolution. Hugoniot measurement of Cu was performed for the demonstration of FES and LRM. For the relation between shock and particle velocities, the fractional standard deviations of the data from the fits range from 0.1 to 0.4 % for copper, and that indicates excellent agreement between our data and the results of the previous studies. Symmetric impact experiment of Au was performed to qualify this material as a high-pressure standard for both dynamic and static experiments. Our data were obtained 0.8 to 3.0 % upward from the previous ones for the back side shock and particle velocities.

2:15PM C5.00003 Equations of State of Selected Armor Ceramics by In-situ High-Pressure X-ray and Ultrasonic Techniques: Comparison with Shock Wave Data, MURLI MANGHNANI, GEORGE AMULELE, ANWAR HUSHUR, University of Hawaii, Hawaii Institute of Geophysics and Planetology, Honolulu, Hawaii 96822 — Ultrasonic measurements of the sound velocity and elastic moduli, and their pressure derivatives for well prepared armor ceramics can provide accurate constraints for establishing their equations of state. Using in-situ high-pressure synchrotron X-ray diffraction and diamond anvil cell techniques at the Advanced Photon Source, we have investigated the compression behavior (V/V0, vs P) for α- and β-SiC, TiB2, B4C, WC and WC-6%Co to 65 GPa. Ultrasonic measurements of Kp and Kvol made to ~15 GPa show excellent agreement with X-ray results. Together, these results are compared with published shock wave data in terms of UJ-Up slope, Kp, compression behavior, elastic anisotropy, and material strength. No phase transition is found in these materials, except for B4C, in which case some structural distortion is indicated.

2:30PM C5.00004 Gruneisen Parameter of Teflon from Hugoniots Measured at Different Initial States, JERRY FORBES, NSWC-Indian Head, PAUL URTIEW, CRAIG TARVER, KEVIN VANDERSALL, Lawrence Livermore National Laboratory — Abstract. The Gruneisen parameter for Teflon is calculated using measured Hugoniot states obtained by shocking Teflon initially at atmospheric pressure and an initial temperature of 200°C. The Gruneisen equation of state is used with the reference state taken as the Teflon Hugoniot measured at atmospheric pressure and an initial temperature of 25°C. An error analysis for Gruneisen parameter γ yields large errors even for carefully done gas gun experiments using manganin gauges. Extremely accurate measurements of pressure, shock velocity, and particle velocity are required to reduce the error in g to approximately ± 10 %.

2:45PM C5.00005 Gruneisen Equation of State for Condensed Media and Shock Thermodynamics, KUNIHITO NAGAYAMA, Kyushu University — Gruneisen equation of state (EOS) for condensed media in terms of pressure, volume and internal energy is suitable for description of high pressure flow problems in condensed media including shock waves. It is shown that thermodynamically formulated Gruneisen EOS can be regarded as a differential equation for internal energy along an isentrope. The differential equation has a formal but general solution for internal energy as a sum of cold part and thermal part. In this solution, the cold internal energy is given by a special solution of the differential equation, while the thermal part is a general solution represented as a product of a function of volume Θ(v) and that of entropy C(S). The volume function can be regarded as a characteristic temperature, Θ(v), whereas the entropy function C(S) is proved to be a conjugate variable of the volume function. The above mentioned formulation is possible under the assumption that the Gruneisen parameter is a function only of volume. Heat added to the system quasi-statically represented as Tds can also be expressed as Θ(v)C(S), which means that the characteristic temperature plays a role of integrating denominator, while C(S) is a conjugate thermal variable with a new integrating denominator. Thermodynamic formulation of the Gruneisen EOS in terms of these new thermal variables has been given. Several examples of the applications of this formulation are also given including (i) compatibility of the formulation with Debye model for the specific heat, (ii) estimation of the variable C(S) along shock Hugoniot, (iii) shock temperature calculation, (iv) Gruneisen parameter calculation by theoretical models, (v) extension to the formulation of anharmonic EOS, etc.

3:15PM C5.00006 Modeling Dynamic Ductility: An Equation of State for Porous Metals, JEFFREY COLVIN, UC/Lawrence Livermore National Laboratory — Enhanced heating from shock compression of a porous material can potentially suppress or delay cracking of the material on subsequent expansion. In this presentation we quantify the expected enhanced heating in an experiment in which a sector of a thin cylindrical shell is driven from the inside surface by SEMTEX HE (peak pressure ~21.5 GPa). We first show the derivation of an analytical equation of state (EOS) for porous metals, then discuss the coupling of this EOS with material elastic-plastic response in a 2D hydrocode, and then discuss the modeling of the HE experiment with both fully dense and 10% porous Ta and a Bi/Ta composite. Finally, we compare our modeling with some recent experimental data.

3:30PM C5.00007 Constitutive Modelling of Shock Compression of a Porous Copper, ANATOLY RESNYANSKY, Weapons Systems Division, Defence Science and Technology Organisation — A substantial number of equations of state have been built up from the Hugoniot data obtained from laboratory and underground nuclear tests. It is generally accepted that testing porous modifications of a material allows researchers to move into the high temperature area of material states. Therefore, the pressure-volume data restored from the porous Hugoniots are very valuable. However, a large amount of the Hugoniots have been obtained from the shock velocity data in a porous samples and in a standard. Primary experimental methods employed for such measurements are time-of-arrival methods, for instance, methods using the pin technique. The present work analyses the data for the material porosity m=4 using a constitutive two-phase rate-sensitive model that was used earlier for description of experimental stress profiles in dry and hydrated sand. The model employs conventional equations of states for the phases of porous copper and available compression curve obtained in independent gas gun experiments. The modelling results demonstrate a good description of the test data.
2:15PM C6.00002 A study of reactive interfaces in Ni+Al particle systems during shock wave propagation, RYAN A. AUSTIN, DAVID L. MCDOWELL, Georgia Institute of Technology, YASUYUKI HORIE, Air Force Research Laboratory, DAVID J. BENSON, University of California, San Diego — Macro-scale responses of energetic materials during shock compression are influenced strongly by thermo-mechano-chemical processes occurring at the level of the microstructure. For example, it is believed that the propagation of chemical reactions in reactive particle systems is intimately linked to conditions at reactive interfaces such as surface temperature, phase changes, defect density, and mass mixing due to inelastic deformation. Mechanistic details of deformation, mass-flow, and mixing, were explored through discrete particle continuum simulations, validated against the experimental measurements. The instrumented gas-gun impact experiments were performed at pressures up to 6 GPa. Based on measured shock velocity increases and shock release characteristics for design of microstructure or materials with controlled energetics.

2:30PM C6.00003 Mechanics driven Chemical Reactions in Structural Energetic Materials, VINDHYA NARAYANAN, DEREK REDDING, Georgia Institute of Technology, SATIHYA HANAGUD, Georgia Institute of Technology — Fundamental mechanistic mechanisms that are responsible for shock-initiation of chemical reactions, are dominated by non-equilibrium processes including changes in reactive particle configurations caused by plastic deformation or by fracture, mixing of constituents in and around the voids, and rapid increases in temperature from mechanical work. Mechanics driven chemical reactions occur in structural energetic materials, during the high-pressure shock state in time scales of mechanical equilibration. These shock-induced reactions represent a unique class of chemical behavior that is not clearly understood. To understand the observed results a model is presented, in this paper, in a hybrid non-equilibrium thermodynamic framework that combines the concepts of internal variables and thermodynamic fluxes. The governing system of partial differential equations is formulated in the framework of extended irreversible thermodynamics. This represents the intimate mixing of the reactants, which is important in the reaction initiation process. The model is developed to distinguish induced or assisted chemical reactions with uniformly blended mixture theories. A yield condition that represents an increase of yield stress behind the shock front is considered. A method of determining the transition states and paths to reach the transition state due to plastic work and void collapse are also discussed. The formulated partial differential equations are integrated and results are discussed.

2:45PM C6.00004 Mechanistic Aspects of Shock-induced Reactions in Ni+Al Powder Mixtures, DAN EAKINS, NAresh THADHANI, Georgia Institute of Technology — A combination of parallel-plate impact experiments utilizing stress measurements and meso-scale numerical simulations are used to investigate the effect of particle morphology on the mechanical and chemical response of Ni+Al powder mixtures. The instrumented gas-gun impact experiments were performed at pressures up to 6 GPa. Based on measured shock velocity increases and shock compressibility changes consistent with the Ballotini model, the flake-based powder mixture was found to exhibit shock-induced reaction. The particle-level mechanistic details of deformation, mass-flow, and mixing, were explored through discrete particle continuum simulations, validated against the experimental results. The micron-scale spherical and flake mixtures were found to display widely varying configurational changes at several length scales, which give insight into why the flake-Ni morphology is more susceptible to shock-induced reactions under the imposed conditions.
4:15PM D2.00002 Simulation of the Richtmyer-Meshkov and Rayleigh-Taylor Instability Using Atomistic Methods
KAI KADAU, JOHN L. BARBER, TIMOTHY C. GERMANN, PETER S. LOMDAHL, BRAD LEE HOLIAN, LANL, BERNI J. ALDER, LLNL — We present large-scale atomistic simulations [molecular dynamics (MD) and direct simulation Monte-Carlo (DSMC)] of fluid instabilities that occur when a fluid interface is subjected to shock loading or gravitation [Richtmyer-Meshkov and Rayleigh-Taylor instability]. The atomistic methods reach the parameter range that is of importance for inertial confinement fusion (ICF) capsules subjected to high energy lasers. The results are compared to existing theoretical and experimental work from which we have strong evidence for the importance of fluctuations in such instabilities. References: 1.) Kai Kadau, Timothy C. Germann, Nicolas G. Hadjiconstantinou, Peter S. Lomdahl *, Guy Dimonte, Brad Lee Holian *, and Berni J. Alder, PNAS 101, 5851 (2004). 2.) K. Kadau et al. submitted (2007).

4:30PM D2.00003 Molecular dynamics simulations of anomalous elastic response of covalent crystals to shock compression
KEITH MCLAUGHLIN, IVAN OLEYNIK, University of South Florida, SERGEY ZYBIN, California Institute of Technology, MARK ELERT, U.S. Naval Academy, CARTER WHITE, Naval Research Laboratory — We have performed large-scale molecular-dynamics simulations of shock-wave propagation in single-crystal covalent solids such as diamond and silicon. An anomalous elastic response of these materials has been observed in the intermediate range of shock-wave intensities between the elastic-plastic split shock-wave regime and the shock-induced chemistry regime. The anomalous elastic response is characterized by the absence of plastic deformations in highly uniaxially compressed material. The unusual response is shock-induced plastic flow and pressure-induced plastic flow.

4:45PM D2.00004 Shock-induced plasticity in bcc metals
BRINGA, J. HAVERLIJK, P. ERHART, H. LORENZANA, Lawrence Livermore National Laboratory, J. WARK, Oxford University — It is often assumed that a shocked material will evolve from a state of uniaxial (1D) strain towards a state of nearly hydrostatic (3D) strain due to shock-induced plasticity. We recently simulated the case offcc copper, where dislocation nucleation and activity leads to a final state close to 3D strain after ∼0.1 ns, as confirmed by simulated X-range diffraction. Simulations with up to 350 million atoms, including defective crystals and ramp loading, were needed to reach such 3D state. This 1D to 3D transition has not been as studied for bcc metals. Although there are several studies of shocks in bcc Fe, a phase transition happens before shock-induced plastic activity appears. We have carried atomistic simulations of shocks in tantalum, using 0.5-50 million atoms, with samples nearly 1 micron long. Our samples include perfect single crystals, defective single crystals, and polycrystals. We find agreement with the experimental Hugoniot up to ∼15% compression, but the complex elastic-plastic shock wave structure does not lead to full 3D relaxation within the 0.2 ns of simulated time.

5:00PM D2.00005 Characteristic cluster size at coalescence following pressure-induced solidification
FRED STREITZ, JIM GLOSLI, DAVID RICHARDS, Lawrence Livermore National Lab — During the initial period of solidifica-
tion, clusters of solid phase nucleate and grow rapidly as liquid is converted to solid. This rapid growth period continues until the clusters coalesce into a connected network and little liquid phase remains. Characterizing the nature of this network of clusters at coalescence is important to understanding the character of the solid at much later times. Using large scale MD simulations of liquid Ta under pressure the solidification process is explored in detail from nucleation to coalescence. We extract growth and nucleation rates from our simulations, as well as cluster size distributions that can be compared against the predictions of simple models. We will show that the length scale for the distribution of cluster size at coalescence is set by the interplay of nucleation rate j and growth rate u. In particular, we find that the characteristic cluster size at coalescence l ~ (a/p)1/4.

Monday, June 25, 2007 3:45PM - 5:15PM – Session D3 Inelastic Deformation I Fairmont Orchid Hotel Plaza 1

3:45PM D3.00001 Embedded Cohesive Elements (ECE) Approach to the Simulation of Spall Fracture Experiment
NICOLA BONORA, LUCA ESPOSITO, ANDREW RUGGIERO, University of Cassino, Italy — Discrepancies between the calculated and observed velocity vs time plot, relatively to the spall signal portion in terms of both signal amplitude and frequency, in numerical simulations of flyer plate impact test are usually shown. These are often ascribed either to material model or the numerical scheme used. Bonora et al. (2003) Bonora N., Ruggiero A. and Milella P.P., 2003, Fracture energy effect on spall signal, Proc. of 13th APS SCCM03, Portland, USA] showed that, for ductile metals, these differences can be the imputed to the dissipation process during fracturing due to the viscous separation of spall fracture plane surfaces. In this work concept that has been further developed implementing an embedded cohesive elements (ECE) technology into FEM. The ECE method consists in embedding cohesive elements (normal and shear forces only) into standard isoparametric 2D or 3D FEM continuum elements. The cohesive elements remain silent and inactive until the continuum element fails. At failure, the continuum element is removed while the ECE becomes active until the separation energy is dissipated. Here, the methodology is presented and applied to simulate soft spall in ductile metals such as OHFC copper. Results of parametric study on mesh size and cohesive law shape effect are presented.

4:00PM D3.00002 Modeling Spallation Damage in Laser Driven Flyer Plate Experiments
DAVIS TONKS, DENNIS PAISLEY, Los Alamos National Laboratory, PEDRO PÉRALTA, Arizona State University, SCOTT GREENFIELD, DARRIN BYLER, SHENGNIAN LUO, DAMIAN SWIFT, Los Alamos National Laboratory, AARON KOSKELO — The TRIDENT laser at Los Alamos has been used to drive small plate impact experiments. Flyers are typically 8 mm in diameter and 0.1 to 1.0 mm thick, while the targets are 10 mm in diameters and 0.2 to 2.0 mm thick. The sample materials are polycrystalline copper and copper composed of large columnar grains. The latter samples reveal information about damage in single crystals and bi-crystals. This work will focus on simulating these experiments to reveal the stress loading histories and to evaluate damage modeling. As part of the former activity, the damage patterns in recovered samples due to edge effects will be explored with a conventional hydrocode and the TEPLA damage model. A crystal plasticity model in the ABAQUS hydrocode will be used to assess the damage seen in the columnar samples. Models of void nucleation at special grain locations and dynamical void growth will be explored.
4:00PM D4.00002 ABSTRACT WITHDRAWN –

5:00PM D3.00006 Temporal Softening and its Effect upon Spall Strength, VICTOR SKOKOV, RFNC-VNIIEF — Experimental observation has revealed that the effects of shock wave loading are extremely complex, often resulting in morphological changes that result in a hardening of the material. Temporal softening that precedes the aforementioned hardening has also been observed. In Al and Cu, the duration of this softening is on the order of 0.3 to 0.5 μs. This work has revealed that, at least in some cases, this temporal softening phenomenon is attributable to the formation of complex bi-periodic twin structures. The overall morphology of these structures is rather complex, consisting of what we shall refer to as “packages,” with each “package” being composed of two sets of parallel twins aligned in a quasi-herringbone pattern. It is probable that the temperature within the “package” is much higher than the temperature of the surrounding material during “package” formation. The formation of bi-periodic twin structures and concomitant temporal softening has an effect upon spall strength. This effect is explored in the work to be presented. Samples are loaded by short duration laser pulses (0.3 – 1 μs) in such a way that the onset of damage occurs within the period of temporal softening. This has enabled an assessment of the softening effect on spall strength.

Monday, June 25, 2007 3:45PM - 5:15PM –
Session D4 Experimental Developments II  Fairmont Orchid Hotel Plaza II

3:45PM D4.00001 Dynamic reflectance measurements of shocked materials1, DANIEL DOLAN, Sandia National Laboratories — Temperature measurements are critical to equation of state development, but are notoriously difficult to perform and interpret. Infrared pyrometry is a valuable temperature diagnostic for a wide range of dynamic compression studies, but the technique is of limited use without knowledge of material emissivity. Although emissivity can be inferred from reflectance measurements — usually at ambient conditions — the manner in which this quantity changes with pressure, temperature, surface condition, and material phase is unknown. This presentation describes an emissivity characterization study of shock-compressed metal films. Real-time, infrared reflectance measurements were performed using light from the VUV ring of the National Synchrotron Light Source to a gas gun system. As the samples are shock compressed, specular reflectance changes are measured using fast near- and mid-infrared detectors capable of tracking individual synchrotron pulses. This research provides data that can be used to constrain dynamic emissivity changes, and may lead to a set of emissivity standards that can be applied to any material.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:00PM D4.00002 ABSTRACT WITHDRAWN –

4:15PM D4.00003 Using Schlieren Visualization to Track Detonator Performance, STEVEN CLARKE, KEITH THOMAS, MICHAEL MARTINEZ, ADRIAN AKINCI, Los Alamos National Lab, MICHAEL MURPHY, RONALD ADRIAN, Arizona State University — Several experiments that are part of a phased plan to understand the evolution of detonation in a detonator from initiation shock through run to detonation to full detonation to transition to booster and booster detonation will be presented. High Speed Laser Schlieren Movies have been used to study several explosive initiation events, such as exploding bridgeworks (EBW), Exploding Foam Initiators (EFI) (or slappers), Direct Optical Initiation (DOI), and ElectroStatic Discharge (ESD). Additionally, a series of tests have been performed on “cut-back” detonators with varying initial pressing (IP) heights. We have also used this diagnostic to visualize a range of EBW, EFI, and DOI full-up detonators. Future applications to other explosive events such as boosters and IHE booster evaluation will be discussed. EPIC Hydrodynamic code has been used to analyze the shock fronts from the Schlieren images to reverse calculate likely boundary or initial conditions to determine the temporal/spatial pressure profile across the output face of the detonator. LA-UR-07-1229

4:30PM D4.00004 The use of silicone based adhesives to encapsulate manganin gauges for high stress experiments, ILAN BE'ERY, ZVI ROSEMBERG, RAFAEL, P.O. Box 2250, Haifa, Israel — The use of commercial manganin stress gauges has been limited to stresses in the range of 0-20 GPa due to the short-circuiting of their encapsulating materials (epoxy, Kapton) at higher pressures. Researchers at Lawrence Livermore overcome this difficulty by embedding their gauges in Teflon sheets and measured shock pressures as high as 40 GPa. The fact that Teflon can keep its resistivity at high pressures is attributed to the lack of benzene rings in its structure. On the other hand, Teflon is difficult to work with as an encapsulating material because of its poor adhesive properties. In order to overcome this difficulty we encapsulated our foils in between two tapes of silicone. Several experiments were conducted in order to directly measure the resistivity of these tapes at high pressures, as well as using them to encapsulate our manganin foils for high pressure studies.

4:45PM D4.00005 The Dynamic Response of Piezoelectric Probes to Low Density Foam Impact, ALAN MEARS, FRANCES BAILY, AWE, Aldermaston, UK, REBECCA STROHMER, Cavendish Laboratory, Cambridge, UK — Small lead zirconate titanate discs within commercial piezoelectric probes were impacted by low density foams in a set of gas gun experiments. For each probe the voltage across a 50 Ohm load was measured to determine the change in electrical charge on the piezoelectric disc. Three different types of foam having densities between 0.1 and 0.35 g/cc were driven at velocities up to 1.0 km/s. Impact with the piezoelectric probes was calculated to generate stresses in the range 0.07 to 0.4 GPa. Hydrocode simulations were run to predict the stress history within the piezoelectric and to interpret the shape of the measured voltage pulse. From the experimental results the piezoelectric charge coefficient d33 was deduced to be around three times the low stress value available for the piezoelectric material. Results for an impact stress of 0.1 GPa followed by pressure release indicate that the dynamic change in polarization has a high degree of reversibility.
5:00PM D4.00006 Magnetoelctric electrode g e - a technique for studying shock compression and matter metallization1, SERGEY GILEV, Lavrentyev Institute of Hydrodynamics, Siberian Division of Russian Academy of Sciences, Novosibirsk, Russia — To study a material, which becomes conductive under compression, we use a new gage of mass velocity. Moving conductive matter generates emf at an electric circuit in transverse magnetic field. Voltage across the electrodes is determined by mean mass velocity at electromagnetic skin-layer in matter behind shock front. Layer thickness depends severly on the electric conductivity of shocked matter and is about 0.1-10 mm for materials investigated. A probing layer travels through the matter with shock velocity giving information on mass velocity under shock wave movement. Unlike the known techniques, the new instrument is Euler gage of mass velocity. Much electrode system allows one to obtain shock velocity at varied spatial bases. This technique is used to build Hugoniot of selenium and aluminum of different density. Experimental data are presented as dependencies of shock velocity on mass one. Thickness of probing layer for coarse powder is about shock transition thickness. This opens up possibilities using the technique for studying structure of shock transition and phase of matter metallization.

3 This work is supported by Russian Foundation for Basic Research, grant 05-02-16398.

Monday, June 25, 2007 3:45PM - 5:15PM –
Session D5 Hydrodynamic and Applied Modeling Fairmont Orchid Hotel Plaza III

3:45PM D5.00001 Numerical Study of Underwater Explosions and Following Bubble Pulses . ATSUHI ABE, MASAHIDE KATAYAMA, ITOCHU Techno-Solutions Corporation, Kasumigaseki Bldg., 3-2-5, Kasumigaseki, Chiyoda-ku, Tokyo, 100-6080, JAPAN, KENJI MURATA, YUKIO KATO, Nippon Koki Co., Ltd. - 2-1, Dobu, Nagasaki, Nishigo-mura, Nishishikawa-gun, Fukushima, 961-8686, JAPAN, KATSUMI TANAKA, National Institute of Advanced Industrial Science and Technology, 1-1-1 Umezono, Tsukuba, Ibaraki, 305-8568, JAPAN — Underwater explosions and following bubble pulses were simulated by using the hydrocode AUTODYN. The pressure gradient depended on the water depth was applied to the water, and the effects of the atmospheric pressure and the gravity on the bubble properties were investigated numerically. In the deep and shallow water depth cases the bubble properties or pressure histories obtained numerically were compared with the empirical formula or the experimental data. Not only the pressure gradient in the water and the atmospheric pressure but also the application of the JWL EOS to slow energy release of the non-ideal explosive (Miller model) were found to be of great importance to simulate the generation of the bubble pulse precisely. Although the gravitational term during the dynamic analysis can be neglected in numerical analyses for very short time phenomena, it is indispensable to simulate the buoyancy of the bubble because the time range of the bubble behavior is some hundred times longer than that of the explosion phenomena.

4:00PM D5.00002 Dynamic Response of Submerged Solids to Extreme Fluid Loading , SHI WEI GONG, MING CHENG, ZHUANGJIAN LIU, CHUN LU, Institute of High Performance Computing, Singapore — This paper deals with the dynamic response of submerged solids to extreme fluid loading induced by underwater explosion. The computational procedure is elaborated for the simulation of charge detonation, shock wave propagation from water media to the target solid, fluid-solid interaction, and dynamic response of the submerged solid. The benchmark tests are conducted, showing that the present method is reasonable and feasible. Cases studies are carried out for a single solid exposed to a single charge detonation or multiple charge detonations; and also multiple solids exposed to a single charge detonation or multiple charge detonations. The effects of different solid geometries on their dynamic responses to underwater explosive loading are also examined. From the results obtained, some insights to the problem of submerged solids subjected to underwater explosive loading are deduced.

4:15PM D5.00003 Modeling of Non-Eroding Penetration Using ALE3D and Zapotec , JAMES CAZAMIAS, UAB, STEPHEN SCHRAML, ARL — Accurate predictions of non-eroding penetration are becoming of increasing importance to the Army. Sandia’s Zapotec (a coupling of Pronto and CTH) has been the code of choice, but there has been some concerns expressed about relying on a single methodology. Consequently, LLNL’s ALE3D (which uses a slide line based approach) is currently being investigated for insertion into ARL programs. While simulations of concrete targets would be preferred for comparison purposes, the current state of concrete models precludes this. As a benchmark, we choose to model the penetration experiments of steel projectiles against aluminum targets (Piekutowski, A.J., et al., Int. J. Impact Engng 23 723-734 (1999)) to examine the differences between the two methodologies.

4:30PM D5.00004 Numerical Modeling of Munroe Jets , CHARLES MADER, Mader Consulting Co., MICHAEL GITTINGS, Science Applications International Corporation — Munroe jets are formed by the oblique intersection of detonation products from two explosive charges separated by an air gap. The jet consists of a high velocity jet of low density precursor gases and particles that travel faster than the primary jet which is a high pressure regular shock reflection. The Los Alamos PHERMEX Data Volumes [1] contain 40 radiographs taken by Douglas Venable in the 1960’s of Munroe Jets generated by Composition B explosive charges separated by 5 to 80 mm of air. In several of the experiments the Munroe jets interacted with thin Tantalum foils and with aluminum plates. The PHERMEX experiments were modeled using the AMR Eulerian reactive hydrodynamic code, NOBEL [2,3]. When the detonation arrives at the bottom of the gap, the detonation product s expand against the air and precursor gases travel at high velocity ahead of the detonation wave in the explosive. The expanding detonation products from the explosive collide and result in a high pressure regular shock reflection. Interaction with a metal plate consists of first the interaction of the precursor gases and then the high pressure regular shock reflection arrives to further damage the metal plate. 


4:45PM D5.00005 Verification Test Problems , BILL Moran, Lawrence Livermore National Laboratory — We present analytic solutions to two test problems that can be used to check the hydrodynamic implementation in computer codes designed to calculate the propagation of shocks in spherically convergent geometry. Our analysis is restricted to fluid media with constant bulk modulus. In the first problem we present the exact initial acceleration and pressure gradient on the outer surface of a sphere subjected to an exponentially decaying pressure of the form \( P(t) = Pe^{-\alpha t} \). We show that very-finely-zoned hydro-code simulations are in excellent agreement with our analytic solution. In the second problem we discuss the implications of incompressible and compressible spherical shells. For the incompressible case, we present the velocity time-history at the inner and outer surfaces of the shell and the radial pressure profile across the shell thickness. We also present a semi-analytic solution to the time-evolution of a nearly spherical shell with arbitrary but small initial 3-dimensional (3-D) perturbations on its inner and outer surfaces. We show that 3-D hydro-code calculations converge to the semi-analytic solution as the resolution increases in the hydro-code. For the compressible case we present the initial conditions that lead to a shock-less acceleration and a time evolution very similar to the incompressible case.

5:00PM D5.00006 ABSTRACT WITHDRAWN –

Monday, June 25, 2007 3:45PM - 5:00PM –
Session D6 Detonation Theory Fairmont Orchid Hotel Promenade I/II
3:45PM D6.00001 JAGUAR Procedures for Detonation Behavior of Silicon Containing Explosives . LEONARD STIEL, Polytechnic University, ERNEST BAKER, CHRISTOS CAPELLOS, WILLIAM POULOS, JACK PINCAY, U.S. Army Ardec, Picatinny, NJ — Improved relationships for the thermodynamic properties of solid and liquid silicon and silicon oxide for use with JAGUAR thermo-chemical equation of state routines were developed in this study. Analyses of experimental melting temperature curves for silicon and silicon oxide indicated complex phase behavior and that improved coefficients were required for solid and liquid thermodynamic properties. Advanced optimization routines were utilized in conjunction with the experimental melting point data to establish volumetric coefficients for these substances. The new property libraries resulted in agreement with available experimental values, including Hugoniot data at elevated pressures. Detonation properties were calculated with JAGUAR using the revised property libraries for silicon containing explosives. Constants of the JWLB equation of state were established for varying extent of silicon reaction. Supporting thermal heat transfer analyses were conducted for varying silicon particle sizes to establish characteristic times for melting and silicon reaction.

4:00PM D6.00002 Porting Initiation and Failure into Linked CHEETAH . CLARK SOUERS, PETER VITELLO, Lawrence Livermore National Laboratory — Linked CHEETAH is a thermo-chemical code coupled to a 2-D hydrocode. Initially, a quadratic-pressure dependent kinetic rate was used, which worked well in modeling prompt detonation of explosives of large size, but does not work on other aspects of explosive behavior. The variable-pressure Tarantula reactive flow rate model was developed with JWL++ in order to also describe failure and initiation, and we have moved this model into Linked CHEETAH. The model works by turning on only above a pressure threshold, where a slow turn-on creates initiation. At a higher pressure, the rate suddenly jumps to a large value over a small pressure range. A slowly failing cylinder will see a rapidly declining rate, which pushes it quickly into failure. At a high pressure, the detonation rate is constant. A sequential validation procedure is used, which includes metal-confined cylinders, rate-sticks, corner-turning, initiation and threshold, gap tests and air gaps. The size (diameter) effect is central to the calibration. This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

4:15PM D6.00003 Effect of Phase Transitions of Chemically Inert Additives on Detonation Properties of Composite Explosives . RAFAEL GUIRGUI, Naval Surface Warfare Center, Indian Head — One-dimensional calculations are used to investigate the effect of phase transitions of chemically inert additives on the detonation properties of high explosives. The resulting small changes in volume of the inert materials can lead to significant changes in the detonation properties when the phase transitions occur within the reaction zone where even the gaseous decomposition products are at high density. The predictions confirm the experimentally observed shift in detonation velocity that occurs when the initial density exceeds a threshold value at which the resulting pressures in the reaction zone correspond to a polymorphic phase transition of the additives. The shift in detonation velocity mostly depends on the sign of the change in volume induced by the transition and to a lesser extent on the sign of the energy released during the transition. Phase transitions causing an increase in volume yield a positive shift in the detonation velocity that is augmented or reduced depending on whether the transition is an exothermic or an endothermic one. The positive shift in detonation velocity is increased when the compressibility of the inert additives is decreased.

4:30PM D6.00004 Monte Carlo Simulations of the Effect of Cross-potential Variations on the Equation of State of N₂/CO₂ Mixtures and of Detonation Products . M. SAM SHAW, Los Alamos National Laboratory — The issues of mixing and cross-potentials were studied with particular emphasis on the implications for detonation products equation of state (EOS) and the prediction of measurable sensitivity to the cross-potential. A large number of Monte Carlo simulations were made with the choice of ensemble depending on the system being studied: NPT for uniform mixing, Gibbs for fluid-fluid phase separation, and Composite for full detonation products with chemical equilibrium and carbon clusters. Simulations with N₂/CO₂ mixtures demonstrate significant sensitivity to the cross-potential in the EOS values for uniform mixtures, in the shape of the isotherms and the location of rapid changes due to fluid-fluid phase separation, and in the location of the fluid-fluid phase separation line in pressure and temperature. Suggestions are made for experimental methods to characterize the cross-potential and mixing properties. Evaluation of the full EOS for HMX based explosives demonstrates an amplified effect of the cross-potential variation through dramatic shifts in thermodynamic equilibrium composition and the resulting EOS.

4:45PM D6.00005 An effect of charged and excited states on the decomposition of FOX-7 . ANNA KIMMEL, Department of Physics, University of Nevada Las Vegas, USA, PETER SUSHKO, ALEXANDER SHLUGER, Department of Physics and Astronomy, University College London, London, UK, MAIJA KUKLJA, Division of Materials Research, National Science Foundation, USA — Various decomposition mechanisms in 1,2-dimino-2,5-dinitrohexane (FOX-7) in both gas and solid phases have been investigated by means of density functional theory calculations using an embedded cluster model. We found that the molecular excitations and charge trapping have a dramatic effect on the decomposition process by facilitating some mechanisms of dissociation and precluding the others: the excited states not only reduce the energetic reaction barriers but also change the type of the dominating chemistry from endothermic to exothermic. We found that the decomposition of FOX-7 in the gas phase is defined by two competing low- energy mechanisms, the C-NO₂ scission and C-NO₂ to CONO isomerisation. Decomposition in solid state of FOX-7 is much more complex and is controlled by cooperative behavior, which involves the excitation processes and structural inhomogeneities in crystalline lattice.

8:00PM - 8:00PM — Session E1 Poster Session l Fairmont Orchid Hotel Salon III

E1.00001 CONTINUUM AND MULTISCALE MODELING —

E1.00002 Discrete Particle Simulation of Shock Compression of Powder Mixtures . DAN EAKINS, ADAM JAKUS, NARESH THADHANI, Georgia Institute of Technology — Numerical continuum simulations have been performed on real, imported powder microstructures, to explore the effect of heterogeneity on changes in configuration during shock compression. A technique has been developed to import two-dimensional micrographs in order to accurately reconstruct the irregular particle sizes, morphologies, and distributions of real powder mixtures. The mechanical response of powder mixtures of widely varying constituent behavior and initial density is investigated at particle velocities of 0.5, 0.75, and 1.0 km/s, through a range of length-scales. Results reveal interesting correlations between powder configuration and micromechanical response during the initial consolidation event. The analysis can be used to design systems for controlled reactions.

E1.00003 ABSTRACT WITHDRAWN —

E1.00004 Reduced Model for Detonation Wave . JEAN-BERNARD MAILLET, LAURENT SOULARD, CEA, GABRIEL STOLTZ, CERMECS — We present a mesoscopic model for reactive waves which extends the model proposed by G. Stoltz (G. Stoltz, Europhys. Lett. 76 (2006) 849). A complex molecule (or a group of molecules) is replaced by a single mesoparticle, evolving according to some Dissipative Particle Dynamics. Chemical reactions can be handled in a mean way by considering an additional variable per particle describing a rate of reaction. The evolution of this rate is governed by the kinetics of a reversible exothermic reaction. Numerical results show that the reactive wave behaves like a detonation wave.

E1.00005 DETONATIONS AND SHOCK INDUCED CHEMISTRY —
E1.00006 Eigenvalue Detonation of Combined Effects Aluminized Explosives. CHRISTOS CAPELLOS, ERNEST BAKER, WENDY BALAS, STEVEN NICOLICH, ARDEC, LEONARD STIEL, Polytechnic University, N.Y. ARDEC TEAM, POLYTECHNIC UNIVERSITY COLLABORATION — This paper reports on the development of theory and performance for recently developed combined effects aluminized explosives. Traditional high energy explosives used for metal pushing incorporate high loading percentages of HMX or RDX, whereas blast explosives incorporate some percentage of aluminum. However, the high blast explosives produce increased blast energies, with reduced metal pushing capability due to late time aluminum reaction. Metal push and dynamic impact experiment work produced during the first few volume expansions associated with cylinder wall velocities and Gurney energies. Our Recently developed combined effects aluminized explosives (PAX-29C, PAX-30, PAX-42) are capable of achieving excellent metal pushing and high blast energies. Traditional Chapman-Jouguet detonation theory does not explain the observed detonation states achieved by these combined effects explosives. This work demonstrates, with the use of cylinder expansion data and thermochemical code calculations (JAGUAR and CHEETAH), that eigenvalue detonation theory explains the observed behavior.

E1.00007 Low Velocity Detonation of Nitromethane Affected by Precursor Shock Waves Propagating in Various Container Materials. HIDEKI HAMASHIMA, Shock Wave and Condensed Matter Research Center, Kumamoto University, AKINORI OSADA, Department of Mechanical System Engineering, Kumamoto University, YUKIO KATO, R&D division, Nippon Koki Co., LTD., SHIGERU ITOH, Shock Wave and Condensed Matter Research Center, Kumamoto University — It is well known that some liquid explosives have two detonation behaviors, high velocity detonation (HVD) or low velocity detonation (LVD) can propagate. A physical model to describe the propagation mechanism of LVD in liquid explosives was proposed that LVD is not a self-reactive detonation, but rather a supported-reactive detonation from the cavitation field generated by precursor shock waves. However, the detailed structure of LVD in liquid explosives has not yet been clarified. In this study, high-speed photography was used to investigate the effects of the precursor shock waves propagating in various container materials for LVD in nitromethane (NM). Stable LVD was not observed in all containers, although transient LVD was observed. A very complicated structure of LVD was observed: the interaction of multiple precursor shock waves, multiple oblique shock waves, and the cavitation field.

E1.00008 A comparison of the blast & fragment mitigation performance of several structurally weak materials. DOUGLAS KIRKPATRICK, ANDREW ARGYLE, KATHERINE HARRISON, JAMES LEGGETT, Defence Science & Technology Laboratory, EDG GROUP TEAM — Structurally weak materials are attractive for explosive blast and fragment mitigation applications because they break up easily into small particles and do not present a secondary hazards. A range of these materials have been investigated under a mitigation research programme aimed at developing a predictive capability. Experiments using 3kg-7.5kg charges confirmed earlier small scale results that porosity and particle density are dominant factors in reducing airblast. Measurement of incident overpressure however, effectively ignores the momentum acquired by the mitigant which has the potential to cause significant damage. Techniques to measure dynamic particle loading have been investigated and initial results are presented. Fragment mitigation performance has been studied with and without the presence of explosive blast. Indications are that for some materials, shock loading from an explosive blast may change the fragment retarding performance. It has also been shown that small quantities of low-density blast mitigant can significantly influence the effectiveness of ballistic protection materials placed close to an explosive.

E1.00009 Mesoscale modelling of PBX. Binder effects. ALEC MILNE, JIM DUNNETT, NEIL BOURNE — In earlier work we have studied aspects of shock to detonation transition and detonation structure in polymer bonded explosives on the scale of the largest grains (the mesoscale) to augment continuum models for these processes. Building blocks have been unreacted Hugoniots of mixtures, mapping from experiment (2D micrographs and 3D tomography) for accurate initial conditions and details of cavity collapse mechanisms as hot spots for ignition. Recently we have applied continuum mixture theory (multi-phase modelling) to dirty binder (the mixture of explosive crystal fines and binder that surrounds the large grains) and validated it for the unreacted Hugoniot of a range of UK explosives. In this paper we build on all of this work and report our progress in using continuum mixture theory to model the reactive behaviour of dirty binder. We begin by considering the binder on its own and then use this continuum mixture model in conjunction with mesoscale representations of PBX. We consider PBX9501 and a UK PBX as examples. We identify the numerical modelling issues that have arisen, our current approaches and our plans for further development and testing.

E1.00010 Development of the wear-resistant composite material containing the diamond powder particle using underwater shock wave. SHIGERU TANAKA, KAZUYUKI HOKAMOTO, SHIGERU ITOH, Kumamoto University — Recently there has been an effort in the development of new composite materials possessing combined properties of high heat conductivity and friction resistant. In this study developing a composite material with such properties using underwater shock wave was attempted. Underwater shock wave can be used to penetrate hard powders into a metal base without decomposition of the base material. In this method, hard powders are penetrates into a soft metal base to obtain a composite with improved surface properties. The purpose of this research is to clarify the experimental conditions for obtaining a new composite material with unique properties. Attempt has been made to obtain aluminum-based and magnesium alloy-based composites by introducing micro/nano-sized diamond particles to the surface of the base metal. The recovered samples showed improvement of wear resistance.

E1.00011 EXPERIMENTAL DEVELOPMENTS —

E1.00012 Improved Temperature Controller System for Gas Gun Targets. S.M. BUCHOLTZ, R.J. GEHR, Honeywell FM&T, R.R. ALCON, R.L. GUSTAVSEN, Los Alamos National Laboratory — Since demonstrating a temperature controller system capable of cooling or heating a gas gun target over the range -75˚C to +120˚C, we have completed 14 gas gun shots with the system. Thirteen of the shots were on the high explosive PBX9502, all cooled to -55˚C. Of the 7.5kg shots we tested, the sample was successfully maintained at temperature for 30 minutes to an hour while other shot preparations occurred. Occasionally, it was necessary to maintain temperature for several hours before shooting. Data from the magnetic gauge used to detect the shock wave suggest that the sample sits while cooling. Calculations yield tilt angles around 10 milliradians. An inexpensive optical system, using the camera already present to observe the system cover plate, has been designed to look for and measure this shift. In addition, improvements have been made to the plumbing for cooling experiments, and modifications have been introduced to improve temperature uniformity and to make the system capable of heating gas gun targets up to +250˚C. This work was supported by the NNSA Enhanced Surveillance Campaign through contract DE-AC04-01AL66850.

E1.00013 ABSTRACT WITHDRAWN

E1.00014 Measuring densities of high-velocity metallic sprays using piezoelectric sensors. CARYS LLOYD, WILLIAM PROUD, University of Cambridge — Recent research efforts in large-scale hydrodynamic experiments have concentrated on the possibility of using piezoelectric sensors to study the evolution of ejecta. Ejecta are small (<100 μm diameter) particulates that are ejected at high velocity (>1 km s⁻¹) from a shocked surface. This paper investigates whether Dynasen PZT piezoelectric sensors are reliable and robust enough to measure accurate time-resolved stresses and densities in high-velocity metallic sprays. The sensors are assumed to have similar characteristics to ejecta sprays, and are generated by a gas gun and in a safe and reproducible manner. A complimentary diagnostic technique, utilising high-speed photography and fast X-ray radiography, measures the densities of the sprays independently, allowing the accuracy of the sensors to be assessed. The Dynasen sensors have been shown to perform relatively well in spray environments. Their accuracy can be improved by taking their mechanical impedance characteristics into account.
E1.00015 A new versatile conductive/radiative heating device for gas gun targets in the 300 K – 500 K range. Capability illustration for analysis of initial temperature influence on shock induced yielding and phase transitions, GILLES ROY, GAEL LANIER, CHRISTOPHE VOLTZ, CEA Valduc, France, FRANCOIS BUY, PATRICE ANTOINE, CEA Valduc — For off-Hugoniot shock loading purpose using existing gas guns, a temperature controller system has been designed to cover the range from 300 K to 500 K for various metals including some featuring low strength or poor thermal conductivity. The heating coil powered by low voltage drives from the impact face the bulk temperature of the target sample typically a few millimetres thick and 40 to 50 mm in diameter. The stainless steel heavy target holder is heated the same way, acting at the periphery as a thermal capacity to limit the thermal losses within the sample. Consequently front and rear sample interfaces remain free for full diameter impact and complete Doppler instrumentation. Typical measurements include DLI and VISAR velocity probing either at free surface or at a LiF window interface. Requested temperature is achieved within 1.5 hour, with an overall gradient better than 5 degrees. Some current applications are illustrated including analysis of temperature effect on TA6V alloy shock induced yielding and Ti allotropic phase transition. The associated issue of LiF properties evolution up to 500 K is also addressed analytically.

E1.00016 The Effect of Sample Preparation on the Release Measurements of Manganin Gauges, DAN THOMAS, DAVID CHAPMAN, WILLIAM PROUD, Cavendish Laboratory, University of Cambridge — Sample preparation and alignment are recognized as essential parts of good experimental practice. As well as close attention to these factors it is also important to recognize that all measurement devices have an inherent resolution time. Depending on the parameter of interest the appropriate degree of sample preparation can be applied. In a previous paper [SCCM 2005] the effect of front surface roughness was compared, in this paper the effect of rear face preparation is addressed. Plate impact experiments on a PMMA sample are described and the stress history measured using Manganin gauges reported.

E1.00017 ABSTRACT WITHDRAWN —

E1.00018 Study of Small Dimension Specimens on SHPB Test, DAWU XIAO, YINLEI LI, SHISHENG HU, University of Science and Technology of China — By SHPB tests combining with theoretical and numerical analysis of series dimension of 2024 aluminium alloy, we concluded that stress-strain curves by specimen of small dimension is reliable. Also an attempt is made to get curves of strain rate over 10^7 s^-1 by small dimension specimen. Accuracy of measurements of transmitted wave is analysed and discussed by experiments and numerical simulation of eccentric compression tests of small specimen. It showed that the distortion of signals can be eliminated by mounting strain gauges in series or far away from the specimen-bar interfaces.

E1.00019 INELASTIC DEFORMATION, FRACTURE, AND SPALL —

E1.00020 Kinetic Behaviour of Failure Waves in a Filled Glass, ANATOLY RESNYANSKY, Weapons Systems Division, Defence Science and Technology Organisation, NEIL BOURNE, School of Mechanical, Aerospace and Civil Engineering, The University of Manchester, UK — Experimental stress and velocity profiles in a lead filled glass demonstrate a pronounced kinetic behaviour of failure waves in the material during shock loading. The present work summarizes the experimental proofs of the kinetic behaviour obtained with stress and velocity gauges. The work describes theoretically this behaviour employing a kinetic model used earlier for a description of fracture waves in pyrex glass. This model is from the family of two-phase strain-rate sensitive models describing behaviour of damaging brittle materials. The modelling results describe well both decay of the failure wave precursor in stress profiles and the velocity attenuation when wave propagating. An influence of the kinetic mechanisms and wave interaction within the test assembly on the reduction of this behaviour is discussed.

E1.00021 More on the response of ceramics to shock waves, ELI BAR-ON, Rafael Ballistics Center — The strength properties of Coors AD995 alumina is investigated in the stress range from about HEL (5 to 7 GPa) and up to 120 GPa. Simulating the experimental work done by Grady, Furnish and Chhabildas and Reinhart and Chhabildas, we try to explain the structure of loading, unloading, reloading and cyclic loadings profiles measured by velocity interferometry. Many physicists are talking about plasticity and slip systems as the mechanism behind the unique structure of the response of Alumina to shock waves, and many use pseudo elastico-plastic strength models to describe this response. Here we try to show that the strength properties of Alumina, being a brittle material, can be derived just from the combined effects of micro-mechanisms like pore crushing and cracks initiation and growth. Any, so called "yield," is due to pore crushing and not to involved slip systems.

E1.00022 Investigations into Spall strengths of geological materials, J.E. FIELD, C.H. BRAINTWAITE, Cavendish Laboratory, Cambridge University, A.R. GUEST, De Beers Group Services, W.G. PROUD, Cavendish Laboratory, Cambridge University — A number of geological materials e.g. hyperbyssal kimberlite, underwent shock loading in a spall configuration to determine the dynamic tensile strength. VISAR was used as the main diagnostic system. As expected the spall strength was found to be significantly lower than the corresponding dynamic compressive or shear strengths but significantly larger than the quasi-static value. It was also found that the visibility of spall signals decreased with increasing sample thickness, this difference being attributed to the progressive comminution of the material.

E1.00023 Dynamic Ductility Measurements of Shocked Metals using Time Sequence Radiography /*This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.*/

1 R.G. GARZA, J.D. MOLITORIS, H.G. ANDRESKI, J.D. BATTEUX, L.M. LAUDERBACH, G.H. CAMPBELL, J.S. STOLKEN, R.L. KRUEGER, Lawrence Livermore National Laboratory, ENERGETIC MATERIALS CENTER / CHEMICAL SCIENCES DIVISION TEAM, MATERIALS SCIENCE AND TECHNOLOGY DIVISION TEAM — Using time sequence radiography we have measured ductility, fracture, and failure of various metals under dynamic shock loading. The metals being examined were in intimate contact with a high-explosive charge that was detonated to produce the transmitted shock. Using high-resolution radiography we obtained a set of images in time sequence detailing how the metal sample responds. Complete data sets to failure were measured for stainless steel and tantalum. As the experiments were designed for single-pass radiography, there are no interference effects. As the samples were shocked directly toward the detectors, fragment mitigation had to be 100% successful. The experimental technique will be presented as well as results on tantalum, stainless steel, and possibly other materials.
E1.0024 Spall Fracture of Metallic Circular Plates, Vessel Endplates and Conical Frustums Driven by Direct Explosive Loads. TETSUYUKI HIROE, KAZUHITO FUJWARA, Kumamoto University, HIDEHIRO HATA, Kumamoto University, DAIKI TSUTSUMI, Kumamoto University — Dynamic fracture experiments are conducted for circular plates, vessel endplates and conical frustums of A2017-7075 aluminum alloys and 304 stainless steel, using a testing apparatus developed applying wire-explosion technique to initiation, where tensile stress waves are generated producing spall in the specimens by the direct incidence of plane detonation waves of the explosive PETN. A VISAR system is adopted to observe the free-surface velocity histories of the specimens. The signals for basic circular plate specimens indicate the characteristics of the failure for tested materials, effects of explosive thickness variations and the configuration of specimens. Hydro-codes are satisfactorily applied to simulate the experimental signal data and observed damage phenomena of recovered specimens. Next, an explosive-filled cylindrical vessel with endplate at the one end is initiated at the other end surface and expanded by axially propagating explosive detonation to fracturing. Both the VISAR signals and numerical simulation indicate a pullback signal of spallation at the endplate. Finally conic frustums are also loaded by plane detonation, showing different type of spall failure due to the additional reflected waves from the sloping side surfaces.

E1.0025 A Study of the Critical Fracture Behavior of High Purity Aluminum in the Dynamic Loading, QI MEILAN, School of Science, Wuhan University of Technology, Wuhan, Hubei, P.R. China, 430070, HE HONGLIANG, Institute of Fluid Physics, CAEP, Miyang, Sichuan, P. R. China, 621900, YAN SHILIN, School of Science, Wuhan University of Technology, Wuhan, Hubei, P.R. China, 430070, SHOCK WAVE AND DETONATION TEAM — One-dimensional shock impact experiments were performed for the High Purity Aluminum — HPA (99.999%). The measurement of free-surface velocity profile and the soft-recovery of the shocked specimen has been obtained at the same time and for the same piece of sample. The critical behavior of HPA in the dynamic tensile fracture has been discussed according to the quantitative metallographic analysis results for the shocked samples. By defining the product of the tensile stress and the time as a parameter called Tensile Impulse, the statistic results indicate that an obvious critical behavior for the damage evolution appears with the increasing of Tensile Impulse. When the Tensile Impulse is low, the damage grows slowly with a linear increment. While once the Tensile Impulse reaches a critical value, the damage grows rapidly and an increment as a power exponential function is observed. Our preliminary results indicate that the critical value of Tensile Impulse for HPA is about 0.34GPa μs. Such a critical transition behavior has been shown by the macro-specimen experimentally for the first time.

E1.0026 A study of the effect of potting voids on the fragmentation of an explosively driven Nitinol Shell. ROBIN MUKERJI, SAM MYERS, GLENN WHITEMAN, AWE — An experimental geometry was designed to determine the effect of potting voids on the fragmentation of a Nitinol ( Ni 55% Ti 45%) Shell. The nitinol shell was subjected to a shock loading using a HE drive such that it would experience an near bi-axial expansion. The region between the HE and the nitinol was filed with a thin layer of potting (Sylgard 184 elastomer), in which two circular voids were positioned. Presented here and results from high speed framing camera and flash x-radiography that were recorded. It was observed that as the shock wave sweeps across the coupon from the centre to the edge, the potting voids cause premature fracture of the nitinol on the outer most point from detonation. The coupon then proceeded to fracture around the void from this point. It is believed that this was due to the build up of detonation products on the outer edge of the void. In addition, a strong effect of the orientation of the fragments was also noticed. This was believed to be due to the directional rolling of the material prior to it being pressed into the coupon.

E1.0027 On the spall strengths and Hugoniot elastic limits of some strong ceramics, ZVI ROSENBERG, YEHEZKEL ASHUAH, RAFAEL, P.O. Box 2250, Haifa, Israel — The dynamic response of strong polycrystalline ceramics is relatively well documented, with high Hugoniot elastic limits (HEL) and very low spall strengths. In contrast, the response of single crystal ceramics is less researched and some of their findings are controversial. In the work presented here we were interested in the extremely high HEL which was reported recently for Gallium Gadolinium Garnet (GGG) as well as in strength of sapphire and magnesium aluminate spinel, on which there are very few reports. The measurements were made with manganin gauges embedded at the back of the specimens, with a thick Plexiglas backing for the gauge. These measured stress-time histories are very simple to interpret and accurate values for the HEL and spall strength of these materials can be easily extracted. Some of our results (e.g. the HEL of GGG) are quite different than those published by other workers.

E1.0028 Two critical damage parameters for the dynamic tensile fracture of ductile metals, HONGHANG HE, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, P.O.Box 919-102, Miyang 621900, P. R. China, YONGGANG WANG, Mechanics and Materials Science Research Center, Ningbo University, Ningbo 315211, P. R. China, MEILAN QI, College of Science, Wuhan University of Technology, Wuhan 430070, P. R. China, FUQIAN JING, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, P.O.Box 919-102, Miyang 621900, P. R. China — A concept of critical fracture in the dynamic tensile spall has been developed via percolation model and two physical parameters, named as the critical linking damage DI and the critical fracturing damage DF, are proposed. DI indicates the critical value of damage for the onset of void coalescence, and DF the critical value for the occurrence of catastrophic fracture. With experimental measurements of the free-surface velocity and the numerical simulations, we demonstrate that these two critical damage parameters are independent on the impact stress and the tensile strain rate, and it is also applicable to predicting the dynamic tensile fracture behavior in metal cylinders. Therefore, we may regard these two damage parameters as the material constants to identify the intrinsic characteristic of the dynamic tensile fracture in explosion and shock wave events.

E1.0029 GEOPHYSICS AND PLANETARY SCIENCE —


E1.0031 Numerical modeling of Deep Impact experiment, V.G. SULTANOV, V.V. KIM, I.V. LOMONOSOV, A.V. SHUTOV, V.E. FORTOV, Inst. Probl. Chem. Phys. RAS — The Deep Impact active space experiment has been done [1,2] to study a hypervelocity collision of a metal impacter with the comet 9P/Tempel 1. The modeling of impact on solid or porous ice made it possible to conclude: the form and size of crater strongly depends on the density of comet material; the copper impacter does not melt and remains in the solid state; the temperature of ejecta varies from 5000 K for solid ice to 15000 K for porous ice. The impact on moist water- saturated sand demonstrated different results. In this case, the copper impacter partly melts, melts, destroys and the ricochet process takes place. In the case of moist porous sand the produced crater is stretched in the direction of impact. The analysis of modeling results indicates to the presence of volatile easy-vaporized chemical compounds in the cometary surface. The hypothesis that the cometary surface consists of only ice does not agree with experimental and computational data on the forming and spreading of impact ejecta. [1] http://deepimpact.jpl.nasa.gov/home/index.html [2] M. F. A’Hearn et al, Deep Impact: Excavating Comet Tempel 1 // Science, 2005, v.310, pp. 258-264
E1.00033 ENERGETIC MATERIALS —


FRANK GARCIA, KEVIN S. VANDERSALL, CRAIG M. TARVER, PAUL A. URTIEW, LAWRENCE LIVERMORE NATIONAL LABORATORY — Shock initiation experiments on the LLM-105 based explosive RX-55-AA (95% LLM-105, 5% Viton by weight) were performed at 25°C and 150°C to obtain in-situ pressure gauge data, run-distance-to-detonation thresholds, and Ignition and Growth modeling parameters. A 101 mm diameter propellant driven gas gun was utilized to initiate the explosive sample with manganin piezoresistive pressure gauge packages placed between sample slices. The run-distance-to-detonation points on the Pop-plot for these experiments showed agreement at 25°C with previously published data on a similar LLM-105 based formulation RX-55-AB as well as a slight sensitivity increase at elevated temperature (150°C) as expected. Ignition and Growth modeling parameters were obtained with a good fit to the experimental data. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

E1.00035 Computational evaluation on the sensitivity of energetic materials

YI LIU, SERGEY ZYBIN, WILLIAM GODDARD, California Institute of Technology — An efficient computational procedure based on molecular dynamics (MD) simulation with ReaxFF reactive force field has been developed to evaluate the sensitivity of various energetic materials including TATB, RDX, PETN, HMX, and TATP. In this study, the two-dimensional slab model is first equilibrated at 300 K, followed by rapid heating up to 2000 K at a rate of 10 K/fs. The system is then allowed to evolve via MD at microcanonical ensemble, where the decomposition of energetic molecules mostly occurs. Another technique mimics the shock impact test and uses two moving wall driving by a constant force to create two impact waves running toward each other, followed by the shock reverberation and material decomposition. Our simulations show that sensitive energetic materials, in general, decompose more quickly than less sensitive ones, which agrees with experimental observations. The chemical reactions found in these simulations are analyzed to understand the mechanisms that account for diverse sensitivity of energetic materials.

Acknowledgements: supported by ARO and ONR grants.

E1.00036 Pressing induced polymorphic phase transition in submicron-sized gamma-HMX

DAVID MOORE, KIEN-YIN LEE, Los Alamos National Laboratory — Submicron HMX has been synthesized and characterized to be less sensitive than impact standard HMX in small-scale sensitivity tests. The sm-HMX was found to be the gamma polymorph and to be stable under ambient conditions for at least a year. Pressing of sm-HMX in a small diameter pellet press at pressures from 10 000 psi to 31 000 psi and 1 to 5 minute hold times was found to promote the gamma to beta polymorphic phase transition. The fraction converted and rate of conversion versus time after pellet removal from the press were found to fit a sigmoidal curve, indicating nucleation and growth as a possible polymorphic transition mechanism.

This work was performed under the auspices of the Joint DoD/DOE Munitions Technology Development Program.

E1.00037 EQUATION OF STATE —

E1.00038 Selection of Reference Material and Type of Its Isentropic Curve in Experiments on Isentropic Compression of Substances in Multi-Megabar Pressure Range

Gennady Boriskov, Nikolay Egorov, V. Timareva, Russian Federal Nuclear Center - VNIIEF — Experimental geometry on isentropic compression of frozen gases in a facility based on a magneto-cumulative generator MC-1 is described. A goal of the experiments is building a “zero” isentropic curve in a pressure range higher 1 Mbar. A radiographing of a studied and reference samples, located in the compression chamber, is carried out during the compression process. A density of the studied sample is determined based on the measured sizes obtained in the result of the x-ray images analysis. Using the sizes of the reference sample and its isentropic curve one can determine the pressure in the studied sample taking into account a gradient correction. Selection of aluminum as the reference material and type of its isentropic curve is explained. The experimental results are compared with the calculation results made using different isentropic curves of Al.

The work was performed in the frameworks of the ISTC project # 2564.

E1.00039 Isentropic Compression of Hydrogen Isotopes Crystal Phase up to 5 Mbar with Ultra-High Magnetic Field Pressure


The work was performed in the frameworks of the ISTC project # 2564.
E1.00040 Software for X-Ray Images Calculation of Hydrogen Compression Device in Megabar Pressure Range¹. NIKOLAY EGOROV, ALEXANDER BYKOV, VALENTY PAVLOV, Russian Federal Nuclear Center - VNIIEF — Software for x-ray images simulation is described. The software is a part of x-ray method used for investigation of an equation of state of hydrogen in a megabar pressure range. A graphical interface that clearly and simply allows users to input data for x-ray image calculation; properties of the studied device, parameters of the x-ray radiation source, parameters of the x-ray radiation detector, the experiment geometry; to represent the calculation results and efficiently transmit them to other software for processing. The calculation time is minimized. This makes it possible to perform calculations in a dialogue regime. The software is written in “MATLAB” system.

²The work was performed in the frameworks of the ISTC project # 2564.

E1.00041 Experiment and Simulations of Ablatively Driven Shock Waves in Gadolinium Metal. RICHARD KRAUS, University of Nevada, Reno, ERIC LOOMIS, SHENNQIAN LEO, Los Alamos National Laboratory, ACHIM SEIFTER, Los Alamos National Laboratory, DAMIAN SWIFT, Los Alamos National Laboratory — Lanthanides are fascinating metals to study because they exhibit physical properties that vary with 4f occupancy. Specifically Gadolinium is interesting because there are multiple structural phase transitions accessible below 100 GPa. Experiments were performed on Gadolinium metal in which shock waves were driven in Gadolinium foils through direct laser ablation. The velocity at the opposite surface of the drive beam was measured with line-imaging laser Doppler velocimetry of the Velocity Interferometer System for Any Reflector (VISAR) type. Simulations of the experiment were done using a radiation hydrodynamic model which takes the measured irradiance history of the laser and predicts the pressure history at the ablation surface; this pressure history is then used as a time-dependant boundary condition for a continuum mechanics simulation. From this we obtain a simulated free surface velocity profile, which we then compare with the velocity profile obtained by the line VISAR diagnostic technique to validate the simulations. With this experimental series we were able to achieve shock pressures up to six gigapascals; specific experimental and simulated results to be presented.

E1.00042 Measurement of the isentropic release data of Au by laser driven shock wave¹. FU SIZU, HUANG XIUGUANG, SHU HUA, WU JIANG, YE JUNJIAN, HE JUHUA, MAN MINXUN, GU YUAN, Shanghai Institute of Laser Plasma — Using the impedance invert-match target coupled with multi-materials, an intense shock pressure was produced in the high impedance material (Au) by high power laser, then its different isentropic release was realized simultaneously in the various low impedance materials (Al, Cu, Zn, Sn, Ag, etc.). On the one hand, using the known EOS of the lower impedance materials, a group of the isentropic release data of Au can be obtained; On the other hand, if the EOS of Au is known, the first shock adiabatic data of all lower impedance materials also can be gotten from the experiment; This can verify systematically the EOS reliability of the various materials. Comparing the two methods of the experimental data processing, the isentropic release curve is more sensitive than the shock adiabat in the systematic verifying of the EOS data. The target manufacture is more difficult, perhaps the target had some distortions when it was employed, and the data from our primary experiment have not the enough precision yet.

¹This work has been supported by 863 National High-Tech Plan of P.R.China

E1.00043 Phonon densities of states of Sn to 64 GPa¹. E.A. TANIS, C. CHEN, H. GIEFERS, X. KE, M. NICOL, M. PRAVICA, University of Nevada Las Vegas, E. ALP, J. ZHAO, Advanced Photon Source, C. GREFF, S. RUDIN, Los Alamos National Laboratory, W. PRAVICA, Wilber Wright College — We measured lattice dynamics of 3 phases of Sn to 64 GPa at ambient temperature by NRIXS and compare the results with DFT computations using the direct force method and all-electron PAW method as implemented in the VASP code. Calculations with either GGA or LDA approximations gave similar results. Other properties calculated from the results include: the Lamb-Mossbauer factor; the mean force constant; vibrational contributions to the Helmholtz free energy; the high and low temperature Debye temperatures; the Debye average phonon velocity; and the Debye-Gruneeisen parameter. At all pressures, experimental and theoretical DOS agree well.

¹The authors thank the XOR team and Michael Lerche for their technical help and U.S. DOE Cooperative Agreement No. FC08-06NA27684 with UNLV for supporting the work. The Advanced Photon Source is supported by the U. S. DOE Office of Science

E1.00044 HIGH ENERGY DENSITY PHYSICS —

E1.00045 Numerical modeling of ferrous cylindrical liners compression. , I.A. MOCHALOV, V.G. SULTANOV, Probl. Chem. Phys. RAS — A method of describing electroconductivity of metal taking into consideration phase transformations for numerical modeling of compression cylindrical liners is proposed and feature of value changing magnetic field induction is considered. Researched assembling consists of two cored cylinders with tiny walls (one inserted into another). External cylinder (impactor - Cu) closely covered by chemical condensed HE. To create magnetic field inside the liner a tiny impulse solenoid is used, which is wound on the conductive liner (Fe). For searching distributions of liner material parameters (pressure, density, temperature) and magnetic field along radius with respect to time for several variants of liner conductivity type were calculated. In addition, phase diagram of realizable states, dynamics of magnetic field changing and temperature of liner internal surface were calculated.

E1.00046 ISENTROPIC AND OFF HUGIONOT LOADING —

E1.00047 Ramp Compression Experiments - Sensitivity of Inverted Isentropes to Experimental Uncertainties. MARINA BASTEA, D. REISMAN, Lawrence Livermore National Laboratory — A wealth of experimental high pressure studies have been aimed in the last decades at understanding the fundamental behavior of matter under compression. Many of them employed well established techniques operating under either static - diamond anvil cell (DAC) or dynamic - shock Hugoniot, high-pressure conditions. More recent technical advancements however made also possible the study of new dynamic regimes by spreading the pressure loading from near-instantaneous, i.e. shock, to tens, hundreds and even thousands of nanoseconds, through the use of laser, electromagnetic and graded density impactor drivers respectively. We present the first sensitivity study of the material isentropes extracted from the ramp compression experiments. We perform hydrodynamic simulations of representative experimental geometries associated with ramp compression experiments and discuss the major factors defining the accuracy of the equation of state information extracted from such data. We discuss the impact of these uncertainties on all platforms. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.
E1.00048 Shockless compression of silicon using high-power laser¹. NORIMASA OZAKI, TOMOKAZU SANO, RYOSUKU KODAMA, TOMOAKI KIMURA, AKIO HIROSE, Graduate School of Engineering, Osaka University, MICHEL KENOIC, LULI, Ecole Polytechnique, KEISUKE SHIGEMORI, DAIGO ICHINOSE, Institute of Laser Engineering, Osaka University — Shockless compression experiments for single-crystal silicon were performed using a high-power laser. Silicon is a typical interesting material exhibiting polymorphism, and the phase diagram is not understood well. For instance, Si is predicted to undergo a metalization transformation under compression. A polycrystalline reservoir target (75 μm) was irradiated with the GEKKO/HIPER laser (λ = 0.35 μm), the reservoir plasma expanding to a vacuum gap (≈ 200 μm) and colliding with a Si sample (20-30 μm). The rear-surface of Si was observed in situ by VISAR (VISAlar) and reflected optical pyrometer. The change of reflectivity from the VISARS may indicate phase transitions under the continuous quasi-isentropic compression. We also for the first time recovered the Si target shocklessly compressed by high-power laser. The structure of the recovered sample was analyzed using a large synchrotron radiation facility.

¹Work supported in part by The Ministry of Education, Culture, Sports, Science and Technology under Grant-in-Aid for Special Purposes No. 18684901

E1.00049 The results of the application of Williamson-Hall procedure for analyses of diffraction maximum broadening of depleted unalloyed macrocrystalline uranium after shock-wave loading in range 20-50GPa. ALEXANDER SHESTAKOV, EUGENY KOZLOV, IGOR ARTAMONOVA, ALBERT NURGALEEV, IRINA PODGORNOVA, EKATERINIA SHESTAKOVA, RFNC-VNIITF — Williamson-Hall procedure for investigation low symmetry lattice sample after shock-wave loading was applied. A number of depleted unalloyed macrocrystalline uranium disks (20mm in diameter, 3mm thick) were used in this testing. The samples under went three different impulse loads of 20GPa, 30GPa and 50GPa. During our registration these loading condition provided the high-speed uniaxial deformation in initial alpha-phase. The state of the preserved uranium samples differed not only in the amplitude and the width of impulse but also in the deformation value, shock heating and the degree of residual temperature. The influence on the samples led to changes in microstructure, including dislocation microstrain. It was shown that the level of the lattice microstrain grew in comparison with its initial states but changed regularly according to the loading conditions. Reducing of uranium crystalline to fragments less then 100nm was not revealed.

E1.00050 Simultaneous determination of Hugoniot and Isentrope in gas gun experiments¹. ROBERT THOE, Lawrence Livermore National Laboratory — We have been exploring the use of the 'reverse ballistics' method to obtain Hugoniot and off Hugoniot Equation Of State. This method uses the unknown sample as the flyer and collides it into a window whose EOS is well known. A VISAR determines the particle velocity which when combined with the windows EOS gives a direct determination of the pressure. Since the pressure and particle velocity are continuous across the interface the shock speed in the flyer can be determined: Us = P/(ρUp). Subtracting the time of arrival of the shock at the back of the flyer from the times of arrival of the rarefaction wave allows the determination of the release isentrope centered at the measured Hugoniot point and extending down to the release pressure as determined by the impendence of the sabot. Besides obtaining both Hugoniot and isentrope data on a single shot, this method has an advantage in that all the timing information is accomplished within the interferometer, i.e. no dependence of cable delays etc.

¹This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

E1.00051 STRESS-STRENGTH MEASUREMENTS —

E1.00052 Explosive Welding of Pipes. 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. 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 water (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. Model experiments with pipes having radii R = 57 mm confirmed results of the calculations and the possibility in principle to weld pipes by explosion with use of water as filler. Reduction of pipe diameter after dynamic loading and explosive welding was ~2%.

E1.00053 The Shock Induced Shear Strength of Polyoxymethylene and Polyethylene. STEPHEN GOVEAS, JEREMY MILLETT, AWE Pic, NEIL BOURNE, University of Manchester — In the past few years, a series of papers has examined the shock response of common engineering polymers to determine their microstructure. In this latest work, the behaviours of two polymers, polyoxymethylene and polyethylene, are investigated under conditions of one-dimensional strain. The study focuses on the experimentally determined lateral component of stress and, from knowledge of the impact conditions, the shear strength. Variations with impact stress amplitude and pulse duration are discussed in terms of the polymer chain structure.

E1.00054 The Response of Dry Limestone to Shock-Loading. DAVE JOHNSON, DAVID CHAPMAN, University of Cambridge, UK, KOSTAS TSEMBELIS, AECL, CA, WILLIAM PROUD, Univeristy of Cambridge, UK — The shock response of geological materials is of interest to many industries, in particular oil and gas exploration. The porous inhomogeneous composition of geological materials complicates characterisation under dynamic loading. The behaviour of dry limestone has been investigated under the condition of uniaxial strain using a plate impact facility. Manganin gauges were used to measure both longitudinal and lateral stresses within the limestone. The Hugoniot and shear data obtained are compared with that available in the open literature.

E1.00055 Twinning and Dynamic Strength of Copper During High-Rate Strain. VICTOR RAEVSKY, RFNC-VNIIEF — The authors will present the results of a study of the conditions under which microstructural changes involving the formation of complex bi-periodic twin structures occurs in copper during shock wave and high strain rate (ε >10⁷ s⁻¹) shock-less loading. The overall morphology of the observed twin structures is rather complex, consisting of what we shall refer to as “packages,” with each “package” being composed of two sets of parallel twins aligned in a quasi-herringbone pattern. The effects of these complex twin structures are also complex. It is widely accepted that deformation twinning results in increased shear strength in samples recovered after shock wave loading. We have observed in this work a significant temporal component to the effect that these complex twin structures have upon shear strength. We have observed, for example, that the formation of these bi-periodic (herringbone-type) twin structures results in an initial loss of shear strength that is significant over a time period of about 0.2 to 0.4 μs. Following the initial loss of shear strength, deformation hardening produces an increase in shear strength that can be as great as several multiples of the initial value.
E1.00056 Tension of Liquids Near Melting Point by Shock Waves , VASYL SOKIV, ALEXANDER UTKIN, VLADIMIR FORTOV, Institute of Problems of Chemical Physics R.A.S.—The influences of strain rate on the negative pressure have been investigated in liquids near melting point by the example of water, hexadecane and pentadecane. The method of spall strength measurements was applied and wave profiles were registered by laser interferometer VISAR. It was cared out in water and hexadecane there is a strong dependence between the strain rate and the registered negative pressure. It is unusual, because ordinarily the negative pressure is almost independent from the value of strain rate, when liquids are far from melting point. It is shown that the double metastable state of water was realized during our experiments. The process of destruction in hexadecane is double staged, like it is in methyl alcohol, unlike in methyl alcohol destruction is double staged only when the loading pressure exceed the threshold of about 250 MPa. At the first stage formation of cavities starts and there is a kinked at free velocity profile was observed. At the second stage the cavity grow rate increases and the spall pulse occurs. Anomalous dependence of the loading pressure on the negative pressure was discovered in pentadecane.

E1.00057 FIRST PRINCIPLES AND MOLECULAR DYNAMICS CALCULATIONS —

E1.00058 Hugoniot of complex fluids from molecular simulation: application to nitromethane , EMERIC BOURASSEAU, CEA-DAM, ANAIS HERVOUET, NICOLAS DESBIENS, JEAN-BERNARD MAILLETT, CEA-DAM, DPTA TEAM —The effect of molecular flexibility on the hugoniot shape is investigated using both MD and MC simulations. In the case of nitromethane, it is shown that molecular deformations with pressure play little role, and thus the rigid approximation may be used. A rigid model potential has then been fitted using a new technique, allowing fitting simultaneously several pressures on the hugoniot curve. This model is then used to simulate the behavior of nitromethane under shock conditions. Results are in good quantitative agreement with experimental data.

E1.00059 Elastic and thermodynamic properties of post-perovskite MgSiO₃ from first-principles calculations , LIU ZI-JIANG, CHEN QI-FENG, CAI LIN-CANG, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, P. O. Box 919-102, China Academy of Engineering Physics, Mianya — The elastic and thermodynamic properties of post-perovskite MgSiO₃ polymorph are investigated at high pressures and temperatures using the plane wave pseudopotential method within the local density approximation. This phase may be the most abundant mineral in the D' region. It is found that the post-perovskite phase has similar bulk modulus and larger shear modulus than perovskite at relevant pressures. The athermal elastic constant tensor of post-perovskite MgSiO₃ are calculated as a function of pressure up to 200 GPa. The calculated results are in excellent agreement with other predictions over the pressure regime studied. The thermodynamic properties of post-perovskite MgSiO₃ polymorph are predicted using the quasi-harmonic Debye model; the heat capacity and thermal expansion coefficient accord with the other calculations at high pressures and temperatures.

E1.00060 MATERIALS SCIENCE —

E1.00061 Current Output from Sandwich-structured Ferroelectric Power Supply , JINMEI DU, GAOMIN LIU, YUSHENG LIU, HAIYAN WANG, YI ZHANG, FUPING ZHANG, HONGLIANG HE — PZT 95/5 ferroelectric ceramics with niobium doped has been assembled for the pulsed power supply, and the electrical current output has been investigated under the action of shock wave in a “normal mode.” The PZT 95/5 ferroelectric ceramics are shocked simultaneously by two shock waves from the two parallel surfaces, so a sandwich-structured ferroelectric power supply is formed. Double current output has been obtained and a high-power electrical pulse over 5 kA is achieved. Theoretical calculation was conducted and a good agreement with the experiment is presented.

E1.00062 Dynamic Shock Compression Response of Ta + Fe₂O₃ Powder Mixtures , DAVID A. FREDENBURG, NAHES N. THADHANI, JOE. COCHRAN, Georgia Institute of Technology — The dynamic shock compression response of stoichiometric and equi volumetric mixtures of varying particle sizes of tantalum and iron oxide powder is investigated to determine their applicability for potential use as a structural energetic material. Compression data gathered in the quasi-static regime is combined with ambient pressure reaction energetics of powder mixtures to determine the optimal mixture configuration for investigation of the dynamic response. Instrumented parallel plate impact experiments are conducted to determine the compaction behavior, reaction threshold conditions, and aid in the development of a heterogeneous compaction model encompassing particle shape, configuration, and individual material properties. This information will be used to study the interactions and stress transfer characteristics in the case of linear cellular alloy structures filled with Ta + Fe₂O₃ powder mixtures upon their impact onto rigid targets.

E1.00063 The Effect of Mechanical Deformation on the Glass Transition Temperature of Polyurea , GILBERT LEE, WILLIS MOCK, JEFFRY FEDDERLY, EDWARD BALIZER, Naval Surface Warfare Center — The glass transition temperature (T_g) of a polyurea was found to be a function of prior mechanical strain and strain rate. Differential Scanning Calorimetry (DSC) measurements were performed on a polyurea following mechanical deformations ranging from low speed tensile testing to high-speed impact from a gas gun. The high-speed impact experiment was done by impacting a steel plate coated with 1/2 inch coating of polyurea with a pointed projectile. The highest strain rates and strain was localized at the center of the plate with the smallest at the circumference. Test specimens were taken from three locations on the coating: at the center free surface, center bounded to steel plate, and circumference (edge). The resulting T_g of the soft domain was found to be, on average, 8°C higher at the free surface than at the bounded surface and 6°C higher than at the circumference. For the low strain rate tensile specimens, the T_g increases with strain and reaches a maximum value at a strain of 3.6. These increases in the glass transition temperatures were interpreted as mixing of the hard and soft segments. The test specimens were subsequently thermally annealed at 100°C. The T_g was found to be about 7°C lower than the previous value. Small angle x-ray analysis has also shown the formation of fibrils in the high strain regions.

E1.00064 High-Strain Rate Response of Ultra-Fine Grained Copper: Experiments and Analysis , A. MISHRA, Dept. of Mechanical and Aerospace Engineering and Materials Science Program, University of California, San Diego, M. MARTIN, N.N. THADHANI, School of Materials Science and Engineering, Georgia Institute of Technology, B. KAD, Dept. of Structural Engineering, University of California, San Diego, M.A. MEYERS, Dept. of Mechanical and Aerospace Engineering and Materials Science Program, University of California, San Diego — Equal Channel Angular Pressing (ECAP) is a severe plastic deformation technique that was used to produce ultra-fine grained copper. The microstructure was optimized using different deformation sequences. A steady state grain size of 200-500 nm was routinely obtained after eight passes (with an effective strain of ∼1 per pass). This resulted in a resulting texture evidenced by EBSD results. The mechanical response was obtained under quasi-static and dynamic conditions. The ultra-fine grained structure produced in Cu by ECAP was found to be thermally unstable. The microstructure recrystallized upon being dynamically deformed due to the adiabatic temperature rise imparted by plastic deformation. This was observed in three modes of high-strain rate plastic deformation experiments: cylindrical and hat-shaped specimens in Hopkinson bar experiments and cylindrical specimens in reverse Taylor impact experiments.
E1.00065 Numerical simulation of the dynamic compaction process for fine iron disilicide powder. ALEXANDER SELEZENEV, VALERY LASHKOV, ALEXEY ALEYNIKOV, OLGA SINKOVA, YURI YANILKIN, RFNC - VNIIEF, Sarov, Russia — Iron disilicide is an attractive material for making thermoelectric generators and temperature sensors. One way to obtain high-density samples of iron disilicide is dynamic compaction technique. The paper summarizes the results of two-dimensional simulation study to optimize the performance of experimental setup for dynamic compaction of fine iron disilicide powder. This optimization was carried out in two-dimensional geometry and used EGAK code. Also, it describes the powder material temperature and pressure values calculated in relation to its loading conditions and initial powder density. The calculation found quantities of the equation of state in Mie-Grüneisen form and the dependence of heat capacity on temperature for crystalline iron disilicide. Elastic pressure versus compression was calculated using ABINIT code, and thermal energy calculation was based on Debye model for the heat capacity of crystal structures. The numerical compaction data were compared against the experimental results.

E1.00066 Shock Characterisation of a Carbon-Fibre Composite, MICHELLE WILLOWS, QinetiQ, Farnborough, UK, WILLIAM PROUD, Cavendish Laboratory, University of Cambridge, PHILIP CHURCH, QinetiQ, Fort Halstead, UK — Composites provide a low-density alternative to many metals and alloys. They are increasingly used as structural components. In this paper carbon fibre re-inforced composite is characterised using a variety of plate impact experiments using VISAR and manganin gauges as diagnostics. The results used to populate a hydrocode model and a ballistic impact scenario is used as a validation experiment.

E1.00067 OTHER TOPICS —

E1.00068 Reduction of steel-ball velocity using sand or water layer accelerated by high explosive (1), TOMOTAKA HOMAE, National Institute of Advanced Industrial Science and Technology, KUNIHiko WAKABAYASHI, TOMOHARU MATSUMURA, YOSHIo NAKAYAMA — The reduction of steel-ball velocity using sand or water was studied. A steel ball, diameter of 9.525 mm, was accelerated using comp. C-4 explosive of 57-52 g. After free flight of about 500-750 mm, the steel ball passed through a sand layer in thickness of 30-125 mm, or a water layer in thickness of 75 or 150 mm. The velocities before and after passage of the layer were determined using a high-speed camera. Although the velocity before the passage was varied from about 300 m/s to about 750 m/s, the velocity after passage was almost constant. The velocity depended only on the kind of materials or thickness of the layer. Sand was more effective in reduction than water for same areal density. Moreover, the steel-ball was accelerated in contact with sand layer in thickness of 30-125 mm. The terminal velocity in such case was comparable to that experienced free flight described above.

E1.00069 Precursor decay anomaly in single-crystal lithium fluoride (2), YUKIO SANO1, TOMOKAZU SANO, Osaka University — The purpose of this study is to demonstrate that the precursor decay anomaly in single-crystal lithium fluoride (LiF) can be reduced using a macroscopic approach. To this end, a method of analyzing the evolving unsteady plane wave fronts created in the crystal upon impact is developed. The values of the parameters included in modeled strain waves in the wave fronts are determined such that the time variation of particle velocity predicted at the impact surface fits the detector current at the surface measured by Asay et al. [J. Appl. Phys. 43, 2132 (1972)]. Another condition is also used that the particle velocity-time histories at and near the surface are initially parallel. It is assumed that when the amplitude of a near-steady precursor in the predicted unsteady wave front, which increases from a static yield stress, becomes a maximum, a kink occurs at the rear of the precursor and then it begins to decay. The precursor decay curves estimated, based on this assumption, are much lower than Asay’s decay curve. These lower curves are expected to reduce significantly the precursor decay anomaly in this crystal.

E1 Professor emeritus of Kobe University of Mercantile Marine

E1.00070 Unsteady state Rankine-Hugoniot jump conditions (3), YUKIO SANO1, TOMOKAZU SANO, Osaka University — A theorem of equivalence regarding the discontinuity of the solution \( \bar{u} = (\bar{u}^{(1)}, \bar{u}^{(2)}, ..., \bar{u}^{(n)}) \) of an underdetermined system of quasi-linear partial differential equations in one spatial dimension is proven. It is also included in the proof that all the thicknesses of the discontinuities of \( \bar{u}^{(i)} \) \( (i=1,2,...,n+1) \) are the same. Unsteady state Rankine-Hugoniot (RH) jump conditions are derived from the system through its integration over the thickness. The jump conditions suggest a possibility that the jumps in \( \bar{u} \) evaluated from the conditions can differ significantly from those from the RH jump conditions. The significant differences in evaluation between both jumps are illustrated by demonstrating that infinitely large jumps in the particle velocity and stress across a spherical wave front are caused by an extremely intense explosion.

E1 Professor emeritus of Kobe University of Mercantile Marine

E1.00071 CAV KO: A simple 1-D Langrangian hydrocode for MS Excel with automatic generation of x-t diagrams, KOSTAS TSEMBELIS1, BEN RAMSDEN, WILLIAM PROUD, Cavendish Laboratory, University of Cambridge, JOHN BORG, Marquette University, Wisconsin, USA — Hydrocodes are widely used to predict or simulate highly dynamic and transient events such as blast and impact. Codes such as GRIM, CTH or AUTODYN are well developed and involve complex numerical methods and in many cases a large computing infrastructure. In this paper we present a simple 1-D Langrangian hydrocode developed at the University of Cambridge, called CAV KO. The motivation being to produce a code which, while being relatively simple, is useful for both experimental planning and teaching the rudiments of code development. Some studies are presented showing the output for a number of scenarios and comparison with experimental results. The code has been adapted from the original KO code written in Fortran by J. Borg, which, in turn, is based on the algorithm developed by Wilkins. The developed GUI within MS Excel and the automatic generation of x-t diagrams allow CAV KO to be a useful tool for quick calculations of plate impact events and for teaching. The code is licensed under the GNU General Public License and can be downloaded from www.shockphysics.com.

E1 Now at - Atomic Energy of Canada Ltd

E1.00072 PHASE TRANSITIONS —
E1.00073 Phase transformation and spall fracture in laser shock-loaded iron. THIBAULT DE RESSEGUIER, MARTINE HALLOUIN, CNRS, LCD TEAM — Despite extensive research work on the α → β phase transition occurring in shock-loaded iron, the kinetics of this transformation remain largely unknown. Here, we present time-resolved free surface velocity measurements in iron foils of thicknesses ranging from 150 to 500 μm subjected to laser shocks of peak pressure about 100 GPa and duration about 5 ns. The records clearly show an elastic precursor followed by a plastic front, but the double wave structure usually associated with the phase change does not appear clearly over such short propagation distances. The measured profiles are compared with the predictions of one-dimensional simulations involving time-dependent descriptions of both twinning and phase transition. Such comparisons provide an estimate of a time constant governing the transformation kinetics, which is found to strongly condition the attenuation of the pressure pulse during its propagation. They also allow testing the predictive capability of simple spall models. Metallurgical observations of the recovered samples confirm both the phase transition and the spall damage inferred from the velocity profiles. Finally, they show the very clear change of fracture surface morphology to the so-called smooth spall expected above the phase transition.

E1.00074 An Estimate for the Deviation from the Mirro Image Due to Solid Liquid Phase Transition of Metals at Shock Unloading. SHLOMI PISTINNERR, Prop. Div. Soreq NRC Yavne Israel, SHARON PEKER, Electrotech Div. Soreq NRC Yavne Israel, MEIR WERDIGER, SHALOM ELIEZER, Prop. Div. Soreq NRC Yavne Israel — We extend the underlying physical reasoning of Walsh and Christian (1955) in a manner which allows a reasonable estimation for the excepted deviation from the mirror image approximation due to solid liquid phase transition. This estimated is limited to a phase transition that occurs at the unloading phase in metals such as Ti and Lead. The idea underlying this estimate is the accumulation of various contributions to the entropy and an estimation of the expected expansion at atmospheric pressure. These estimates combined with the Lindmann melting law and the Clausius Clpyeron equation are used to estimate the expansion at the phase transition and the resulting change in free surface velocity.

E1.00075 Phase transitions of C_{70} fullerite under step-like shock compression. SERGEY SOKOLOV, VLADIMIR MILYAVSKYI, TATIANA BORODINA, VLADIMIR FORTOV, IHED of JIHT RAS — Shock-induced phase transitions of C_{70} fullerite were studied with use of recovery assemblies of planar geometry at pressures 8 to 52 GPa. Two types of starting material were investigated: polyphase [1] and monophase C_{70} withhcp-structure. We have found that the results of shock-wave compression of fullerite C_{70} with various initial phase compositions qualitatively coincide in all explored pressure range. Rhombohedral modification of C_{70} completely disappears already at pressure 9 GPa. At the same time, crystalline modification of C_{70} with hcp-structure in conditions of step-like shock-wave compression does not undergo phase changes down to 9 GPa and practically completely disappears from the recovered material only at 23.5 GPa. Shock-induced transformation of hcp into fcc structure was fixed at pressures in the range 9 to 23.5 GPa. Depth of this transformation is increasing with growth of shock pressure. In the specimens recovered from 23.5 GPa, the only crystalline phase of fullerite C_{70} with fcc structure is observed (about 5 %) and for the first time transformation of a graphite-like carbon is fixed (about 95 %). With growth of shock pressure up to 26 GPa and higher, destruction of C_{70} molecules occurs. The work was supported by RFBR and RSSF. [1] V.V. Milyavskyi, T.I. Borodina, S.N. Sokolov, A.Z. Zhuk. Diamond and Rel. Mat. 14 (2005) 1924.

E1.00076 Hugoniot and phase transition in silicon nitride porous samples. VLADISLAV YAKUSHEV, ALEXANDER UTKIN, ANDREY ZHUKOV, Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia — In this work by laser interferometer VISAR investigated the behavior of silicon nitride porous samples with porosity of ~15% in high pressure shock waves in the region of 15 – 50 GPa. Hugoniot was constructed. The interest to the high density c- modification mainly caused by its hardness, close to hardness of cubic boron nitride and diamond. In this work we investigate the phase transition from β-Si3N4 to c-Si3N4 in porous samples by laser interferometer method for sample surface velocity registration. This method allows to obtain with high resolution mass velocity profiles of sample material at shock compression. The analysis of structure of such profiles gives the information about phase transition and its kinetics. Also by results of experiments Hugoniot is constructed. Having Hugoniots at different porosities allows to construct equation of state with maximal accuracy, which define the phase balance curve, in this case, balance between β- and c- phases.

E1.00077 SPECTROSCOPY AND OPTICAL STUDIES

E1.00078 Study of the laser-induced decomposition of HNO3/ 2-Nitropropane mixture at static high pressures. VIVIANE BOUYER, PHILIPPE HÉBERT, MICHEL DOUCET, CEA/DAM — HNO3 / 2-Nitropropane is a well known energetic material on which Raman spectroscopy measurements at static high pressure in a diamond anvil cell (DAC) have already been conducted at CEA/LE RIPAULT in order to examine the evolution of the mixture as a function of composition and pressure [1]. The purpose of the work presented here was to study the laser-induced decomposition of these energetic materials at static high pressures by measuring the combustion front propagation rate in the DAC. First of all, the feasibility of the experimental device was checked with a well known homogeneous explosive, nitromethane. Our results were consistent with those of Rice and Foltz [2]. Then, we investigated the initiation of NA / 2NP mixture as a function of nitric acid proportion, for a given pressure. We chose the mixture for which both the combustion propagation rate and detonation velocity are maximum and we examined the evolution of the front propagation velocity as a function of pressure and energy density. [1] Hebert, P., Regache, I., and Lalanne, P., “High-Pressure Raman Spectroscopy study of HNO3 / 2-Nitropropane Mixtures. Influence of the Composition.” Proceedings of the 42nd European High-Pressure Research Group Meeting, Lausanne, Suisse, 2004 [2] Rice, S.F., et al., Combustion and Flame 87 (1991) 109-122.

E1.00079 Temporal change of Raman spectra of carbon tetrachloride under laser-driven shock compression. KUNIHIKO WAKABAYASHI, TOMOHARU MATSUMURA, YOSHIO NAKAYAMA, Research Center for Explosion Safety, National Institute of Advanced Industrial Science and Technology (AIST), EISUKE YAMADA, MITSUO KOSHI, Department of Chemical System Engineering, School of Engineering, The University of Tokyo — Nanosecond time-resolved Raman spectroscopy has been performed to study a molecular response of carbon tetrachloride under laser-driven shock compression at laser power density of 5 GW/cm^2. Shock wave was generated by using the glass-confined geometry target. Intense Raman bands of CCl4 at 460 cm^{-1} showed red shift (18 cm^{-1} at maximum), and its intensity increased along with the propagation of shock wave. The anti-Stokes and Stokes ratio increased during shock compression due to the shock induced temperature rise. The relationship between the change of Raman band and the propagation of shock wave will be discussed by using the hydraulic simulation and the measured particle velocity of shock compressed CCl4.

E1.00080 Simulating Picosecond X-ray Diffraction from Shocked Crystals using FFT Methods on MD Output. GILES KIMINOU, ANDREW HIGGINBOTHAM, WILLIAM MURPHY, JUSTIN WARK, University of Oxford, UK, JAMES HAWRELIAK, DAN KALANTAR, HECTOR LORENZANA, BRUCE REMINGTON, LLNL, NIGEL PARK, AWE, Aldermaston, UK — Multi-million atom non-equilibrium molecular dynamics (MD) simulations give significant insight into the transient processes that occur under shock compression. Pico-second X-ray diffraction enables the probing of materials on a timescale fast enough to test such effects. In order to simulate diffraction patterns, Fourier methods are required to gain a picture of reciprocal lattice space. We present here results of fast Fourier transforms of atomic coordinates of shocked crystals simulated by MD, and comment on the computing power required as a function of problem size. The relationship between reciprocal space and particular experimental geometries is discussed.

The work was supported by RFBR, grant number 06-03-33138, and Russian Science Support Foundation.
8:00AM F1.00001 Analyzing Isentropic Compression Wave Experiments. DENNIS B. HAYES, Sandia National Laboratories, Albuquerque NM 87185. Some common assumptions that are used to analyze shock wave experiments are invalid for analyzing ramp wave compression experiments. One example is the analysis of a Doppler shift through a window using a steady wave in the window, a condition that is violated when a ramp compression wave steepens as it propagates, requiring separate consideration during the analysis (LiF to 20 GPa). Introduction of a free or windowed interface produces large perturbations to the flow in the sample that must be reconciled to achieve required timing accuracy; when the specimen has a unique stress-strain compression relation, the equations of motion are hyperbolic so that stress-strain relation can be directly deduced from measurements on two samples (sapphire to 20 GPa). The sample is hysteretic like an elastic-plastic material, there is not a unique solution to the flow and a separate drive measurement is needed (W to 250 GPa). Time-dependent plasticity (spall in aluminum or twinning in U6Nb) has parabolic equations and backward solutions are unstable. Analyses that compare experiment and simulation have very broad minima in the parameters used to model stress-strain. Unconstrained polynomial expansions can wander and converge to unreasonable results. Better convergence is achieved with constrained models like certain forms of the Mie-Grüneisen EOS (Cu to 18 GPa) but those poorly represent materials with large changes in compressibility with strain (HMX to 50 GPa or β-γ phase change in Sn at 5-8 GPa). Maintaining small sample thickness to eliminate shock-up while maximizing thickness for accurate wave velocity measurement produces problems for designing high-stress experiments and leads to hybrid experimental designs.

9:00AM F1.00003 New experimental capabilities and theoretical insights of high pressure compression waves. DANIEL ORLIKOWSKI, Lawrence Livermore National Laboratory — Laser produced x-ray drive was used to shocklessly compress solid Al, Ta, W, V and C targets to high peak longitudinal stresses over nanosecond timescales. Interface velocities versus time for multiphase samples were measured and converted to stress-density for near isentropic conditions using an iterative Lagrangian analysis. These are the most rapid shockless compression stress-density data ever reported. Stress-density is stiffer than expected from models that are benchmarked against both static and shock experiments, suggesting a larger than expected time dependent viscoelastic response. This time-dependent compression applied to Bi, Si and Fe samples results in multi-structural phase transformations. A time resolved velocity interferometer is used to measure the effects of new phases on a transmitted wave velocity profile yielding insights into the transformation kinetics. With different experimental techniques, it is now possible to vary the dynamic compression rise time applied to a given material by 10 orders of magnitude. This capability of varying the ramp compression timescales enables the study of time-dependent material behavior associated with structural changes and deformation in solids subjected to extreme compression.

1 Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:30AM F1.00004 PANEL DISCUSSION — Tuesday, June 26, 2007 10:30AM - 12:30PM — Session G2 Material Science I Fairmont Orchid Hotel Amphitheater

10:30AM G2.00001 High-pressure phase synthesis of Si using femtosecond laser-driven shock wave. TOMOKAZU SANO, MASASHI TSUJINO, NORIMASA OZAKI, TOMOAKI KIMURA, RYOSUKE KODAMA, AKIO HIROSE, Graduate School of Engineering, Osaka University, Japan, OSAMI SAKATA, Japan Synchrotron Radiation Research Institute / SPring-8, MASAYUKI OKOSHI, NARUMI INOUE, National Defense Academy of Japan — High-pressure phases of silicon are synthesized using femtosecond laser-driven shock wave. The crystalline structure in a recovered sample was determined using synchrotron x-ray diffraction and electron diffraction methods. The high-pressure phase with simple hexagonal structure exists in the recovered sample. The metastable BC8 structure also exists. The temperature profile in the shock wave as a function of the pressure was estimated using the thermodynamic theory. The estimated results agree well with the experimental results.
10:45AM G2.00002 Dynamic mechanical behavior of boron carbide-based composites. SHMULIK HAYUN, NAHUM FRAGE, MOSHE DARIEL, EUGENE ZARETSKY, Ben-Gurion University, Israel. —This presentation is concerned with the dynamic response of two types of boron carbide-based composites. The composites were fabricated by infiltration of compacted but unsintered B$_4$C preforms and of partially sintered B$_4$C skeletons by liquid Si. During the infiltration process, molten silicon reacts with the B$_4$C phase resulting in the formation of the SiC and B$_4$C(B,C,Si)$_3$ phases. Some residual silicon is also present in the infiltrated composites. The dynamic behavior was studied in planar impact experiments (impact velocities 100-1000 m/sec) using a 25 mm gas gun. The velocities of the sample-Polyurethane window interface were monitored continuously by VISAR. The composites failed completely in compression, at loads above their HEL (17-18 GPa). The spall strength, deduced from low-velocity impacts, ranged from 0.5 to 1.1 GPa, depending on the tensile strain rate. Scanning electron microscopy (SEM) with energy dispersive spectrometry (EDS) were used to analyze the fracture surface. The correlation between the microstructure of the infiltrated composites and their dynamic response is discussed.

11:00AM G2.00003 Shock compression properties of hard materials, TSUTOMU MASHIMO, Kumamoto University. — Through the measurement of Hugoniot parameters, we can get useful information about high-pressure phase transition, equations of state (EOS), etc. of solids, without pressure calibration. We have performed the Hugoniot-measurement experiments on various kinds of hard materials of calcogenides, oxides, nitrides, borides by using a high time-resolution streak camera system (inclined-mirror method) to investigate the yielding property, phase transition and EOS. It was found that almost all brittle materials behave as an elasto-isotropic solid unlike metals (elasto-plastic solid), except a very few materials such as Tl$_2$. We observed the shock-induced phase transitions on ZnS, ZnSe, TiO$_2$, ZrO$_2$, Gd$_2$Ga$_5$O$_{12}$, AlN, B$_4$C, etc. Some oxide materials showed virtually incompressible EOS's in the high-pressure phase region. Here, the Hugoniot-compression data are reviewed, and the yielding property, phase transition and EOS of these hard materials are discussed. The applications for anvil materials, shock-resisted materials, etc. are also discussed.

11:30AM G2.00004 Comparison of High Strain Rate Properties of Tantalum Processed by Equal Channel Angular Pressing, PHILIP FLATER, JOEL HOUSE, Air Force Research Laboratory, JAMES O'BRIEN, O'Brien & Associates, WILLIAM HOSFORD, University of Michigan. — Current ingot refinement and solidification techniques used in tantalum processing often result in inconsistent mechanical properties. Subsequent processing by equal channel angular pressing (ECAP) has been shown to reduce or eliminate internal structural variations as well as part-to-part variability [Hartwig, 2006]. This paper investigates the effects of ECAP processing on the properties of tantalum. The materials of interest are 2.5-inch round bar tantalum supplied by H.C. Starck and Cabot Supermetals. Three metallurgical conditions were examined for each material: as worked, fine-grain annealed, and large-grain annealed. Prior to annealing, each bar was processed eight times through a 135 degree ECAP die using route Bc then forged into 0.25-inch plates. Specimens were then removed from the plates. Mechanical properties were evaluated using low- and high-rate uniaxial compression experiments. Specimen load axis were oriented either through-thickness or in the plane of the original plate. Wave propagation and anisotropy were studied using the Taylor impact experiments. The experimental results and physical and mechanical characterization will be discussed.

11:45AM G2.00005 Shock compression of magnesium silicon nitride, TOSHIMORI SEKINE, TAKAMICHI KOBAYASHI, National Institute for Materials Science, BERT HINTZEN, Eindhoven University of Technology. — Magnesium silicon nitride is a ternary nitride compound with an orthorhombic, distorted wurtzite structure at ambient condition. There is no study on this material at high pressures, but a recent theoretical work predicts phase transitions at ~17 GPa. We have determined Hugoniot for magnesium silicon nitride ceramics up to 150 GPa and performed recovery experiments up to ~50 GPa. The Hugoniot measurement indicates HEL of 15-17 GPa and a compression curve with no clear phase transition. The compression curve, however, showed a gradual deviation from the compression curve calculated for the low-pressure phase with increasing pressure. If this is the case, there would be a sluggish phase transition at high pressure. We carried out a series of recovery shots on the powders mixed with copper, but the results indicated no additional phase. We compared the results with the theoretical prediction.

12:00PM G2.00006 Laser-induced damages to sapphire single crystals, PEDRO PERALTA, SHENG-NIAN LUO, Los Alamos National Lab, CHI MA, California Institute of Technology, DENNIS PAISLEY, Los Alamos National Lab — Sapphire (α-Al$_2$O$_3$), an important optical material, has often been used as a substrate or window in laser-induced shock wave loading of condensed matter. Systematic experiments were conducted to investigate its breakdown threshold, spall and fracture, plasticity, melting and recrystallization, upon μs laser pulse illumination on the (0001) surface (wavelength of 1054 nm). One of the surfaces of the cylindrical sample was examined with microsectic optical techniques. At sufficient laser fluxes, fracture was induced; the fracture patterns on the uncoated surface correlated with the spatial distribution of the driving pulse, and demonstrated three-fold symmetry as expected for the (0001) surface. Plastic deformation and solid–solid phase change were also characterized. On the coated side, the ultrafast heating and quenching yielded melting, vitrification, and nanocrystalline hexagonal and cubic phases.

12:15PM G2.00007 Phase transitions, high-rate straining and fracture of iron under spherical explosive loading, A.V. PETROVTSEV, E.A. KOZLOV, C.A. BRICHIKOV, V.V. DREMOV, G.V. KOVALENKO, D.A. VARFOLOMEEV, FRCN-VNIITF, Russia, A.M. BRAGOV, A.K. LOMUNOV, RIM, NNGU, Russia, A.V. DOBROMYSLOV, N.I. TALUTS, IMP, RAS, Russia, A. JUANICOTENA, M. KOBAYASHI, National Institute for Materials Science, BERT HINTZEN, Eindhoven University of Technology. — Magnesium silicon nitride is a ternary nitride compound with an orthorhombic, distorted wurtzite structure at ambient condition. There is no study on this material at high pressures, but a recent theoretical work predicts phase transitions at ~17 GPa. We have determined Hugoniot for magnesium silicon nitride ceramics up to 150 GPa and performed recovery experiments up to ~50 GPa. The Hugoniot measurement indicates HEL of 15-17 GPa and a compression curve with no clear phase transition. The compression curve, however, showed a gradual deviation from the compression curve calculated for the low-pressure phase with increasing pressure. If this is the case, there would be a sluggish phase transition at high pressure. We carried out a series of recovery shots on the powders mixed with copper, but the results indicated no additional phase. We compared the results with the theoretical prediction.

Tuesday, June 26, 2007 10:30AM - 12:15PM
Session G3 Inelastic Deformation II
Fairmont Orchid Hotel Plaza I

10:30AM G3.00001 Effects of Processing Techniques on the Shock Response of Be, ERIC LOOMIS, SHENGNIAN LUO, DAMIAN SWIFT, SCOTT GREENFIELD, DENNIS PAISLEY, RANDALL JOHNSON, Los Alamos National Laboratory. — Microstructural effects including material anisotropy, impurities, grain size, and texture alter a materials response to dynamic loading through wave front dispersion and inelastic processes. The spatial variations created by these effects may ultimately prevent significant energy gain from being attained with inertial confinement fusion (ICF) due to instability seeding if they are not minimized through material processing. To this end, laser-driven confined shock experiments have been conducted on Be to characterize its dynamic strength properties and usefulness as a possible ICF ablator. Disks of Be 3 mm in diameter and 100 to 250 microns thick in the form of single crystal, rolled foil, equal channel angular extruded, and sputtered Be-Cu were dynamically loaded to 100’s kbar while the material behavior was measured at most locations. Fine two-wave structures were observed in free surface velocity records providing a comparison of flow stress and other dynamic properties between Be types. 2-D continuum mechanics simulations were used to elucidate the underlying physics involved in the dynamic material response of the shocked Be.
10:45AM G3.00002 Dynamic Compression of a Zr-Based Bulk Metallic Glass Confined by a 304 Stainless Steel Sleeve1, MORGANA MARTIN, Georgia Institute of Technology, LASZLO KECSKES, Army Research Laboratory, NARESH THADHANI, Georgia Institute of Technology — We will report on our current work on dynamic high-strain-rate mechanical properties of a zirconium-based bulk metallic glass (LM106m) with and without a stainless steel confinement sleeve. The dynamic compression experiments were conducted using reverse Taylor anvil-on-road impact tests to generate strain rates of ∼10³ s⁻¹. High-speed digital photography was used to obtain transient images of the deformation history. Velocity interferometry was also used to determine the back surface velocity of the impacted rod-shaped sample. These tests provide qualitative and quantitative information about the transient deformation and failure response of the specimens, which is used to better correlate the deformation path with the final recovered geometry. The recovered impacted specimens were analyzed using microscopy and AUTODYN modeling to elucidate the deformation and failure mechanisms of the bulk metallic glass and the effects of the altered stress state caused by the confinement sleeve. In this paper, the dynamic compression results and corresponding analysis of the failure mechanisms will be presented.

Funded by ARO Grant No. E-48148-MS-000-05123-1 (Dr. Mullins program monitor) and a NASA Jenkins Fellowship.

11:00AM G3.00003 Dislocation Patterning and Dynamic Fracture in Shock-Loaded Tantalum and Uranium Alloys, LUKE HSIUNG, Lawrence Livermore National Laboratory — Deformation substructures in fragments of bcc metals and alloys: Ta, Ta-2.5%W, Ta-10%W, and U-6wt%Nb recovered from HE-driven shock experiments; all were conducted under a peak pressure of ∼30GPa, were characterized and analyzed using transmission electron microscopy (TEM) techniques. The relationships between dislocation patterning and dynamic fracture mode of the fragments are correlated. The results reveal that dynamic damage and fracture in bcc metals are intimately related to the reactions for dislocation patterning, such as deformation twinning and the formation of cell walls or sub-boundaries, which in turn are governed by the mobility of dislocations under dynamic-pressure conditions. Deformation twinning phenomenon becomes significantly enhanced in U-6Nb containing high-density and low-mobility dislocation patterning, such as deformation twinning and the formation of cell walls or sub-boundaries, which are governed by the mobility of dislocations under dynamic-pressure conditions. The embrittlement of U-6Nb under dynamic-pressure conditions is found to mainly be caused by the structural instability and the mutual collision of twin bands, which lead to the enhancement of spall-like damage. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

11:15AM G3.00004 Shock Wave Profile and Bauschinger Effect in Depleted Uranium1, DARCIE D. KOLLER, GEORGE T. GRAY III, Los Alamos National Laboratory — Bauschinger effect is observed in many metals and is characterized by a microstructural stress distribution that results in an increase in compressive yield strength at the expense of tensile yield strength. Experiments to explore this phenomena are accomplished by applying a stress to the specimen in one direction to the yield point and then reversing the direction of the applied stress to the same magnitude. When the loading is applied in the negative direction, materials displaying the Bauschinger effect will yield before reaching the same load that yielding occurred at in the positive direction. This series of experiments applies uniaxial compressive loading followed by uniaxial tensile loading (negative direction of compressive load) by means of plate impact experiments on depleted uranium samples. Wave profiles are observed with VISAR to compare the HEL during the compressive loading with the HEL seen during release while the sample undergoes tensile loading. The expected 2 wave structure (elastic-plastic behavior) is observed during the compressive loading (shock up), but this structure is diminished on the release portion of the wave profile indicating a diminished yield strength during the tensile loading.

LA-UR-07-1151

11:30AM G3.00005 Influence of Microstructure on the Bauschinger Effect and the Shock Hardening in 1080 High-Carbon Steel, GEORGE GRAY III, ELLEN CERRETA, LISA DOUGHERTY, CARL TRUJILLO, MIKE LOPEZ, Los Alamos National Laboratory — The importance of a microstructurally-controlled Bauschinger component to defect storage during the shock loading process has been shown to be correlated to both quasi-elastic release effects and reduced shock hardening in materials. In the current study shock recovery experiments have been conducted on a high-carbon 1080 steel as a function of two microstructural states; fully pearlitic and where the cementite has been spheroidized. The 1080 steel in the fully-pearlitic condition is shown to exhibit a significant Bauschinger effect while the spheroidized microstructure is observed to display significantly higher shock hardening when shock pretrained to an equivalent shock peak stress. The shock hardening response of 1080 steel is discussed in terms of the micromechanisms controlling defect generation and storage during shock loading in materials.

11:45AM G3.00006 Failure above and below the elastic limit in AD995, NEIL BOURNE, University of Manchester, JEREMY MILLETT, AWE, Aldermaston, M.W. CHEN, Tohoku University, DATTA DANDEKAR, JAMES MACCAULEY, ARL, Aberdeen — There is an ongoing interest in identifying inexpensive armour materials for use in protection of personnel and vehicles. The response of AD995 under shock loading is one of the materials most extensively investigated. Over recent years, workers have reported failure occurring in various polycrystalline ceramics behind the shock front. This phenomenon has been investigated using embedded stress sensors and a recovery technique that has allowed observation of the microstructure above and below the HEL and these results are brought together here to explain the observed behaviour. The failure front velocity is found to change with the applied stress, in particular it slows markedly as the HEL is exceeded. The evidence in the microstructure shows the response below HEL is dominated by intergranular failure whilst above HEL the response dominated by plasticity in grains (including twinning), which alters failure characteristics.

12:00PM G3.00007 ABSTRACT WITHDRAWN —

Tuesday, June 26, 2007 10:30AM - 12:30PM —
Session G4 Isentropic and Off Hugoniot Loading
Fairmont Orchid Hotel Plaza II

10:30AM G4.00001 Making and Characterizing Off-Hugoniot States in Gas Gun Experiments, JEREMY PATTERSON, Lawrence Livermore National Laboratory — Understanding the high-pressure, high-temperature behavior of materials subjected to dynamic loading requires knowledge beyond typical Hugoniot EOS and sound speed experiments. Recent advances in the fabrication of Graded Density Impactors (GDIs) have enabled us to produce both smooth, continuous quasi-isentropes and complex tailored compression paths. In addition we have developed ellipsometry as an in-situ real-time diagnostic capable of measuring optical constants during gas gun experiments. Since measured optical constants can be related to crystal structures as well as emissivities, coupling ellipsometry with GDIs provides a means to create and characterize a wide region of thermodynamic space previously inaccessible in standard shock experiments. We present quasi-isentropic compression of Ta to over 1 Mbar, and ellipsometry measurements of solid-solid and solid-liquid phase transitions as well as pressure-induced solidification of water.

1This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.
numerical schemes to reproduce the physical features. We illustrate them on the example of a virtual material which gathers all these cases. Hydrocode calculations based on this material show the difficulties of introduces isentropic compression waves in the middle of shock waves and released shocks in the middle of expansion fans. After basic phenomena explanations, we show that decrease of the sound speed can occur in the general case when a wave propagates through a material with a non convex equation of state. We show that decrease of the sound speed introduced by Menikoff, Brun and their co-authors, but the general case remained to be explained. Our purpose is to provide the explanation of the successive waves which occur in the general case when a wave propagates through a material with a non convex equation of state. We show that decrease of the sound speed introduces isentropic compression waves in the middle of shock waves and released shocks in the middle of expansion fans. After basic phenomena explanations, we illustrate them on the example of a virtual material which gathers all these cases. Hydrocode calculations based on this material show the difficulties of numerical schemes to reproduce the physical features.

HEUZE, STEPHANE JAOUEN, HERVE JOURDREN, CEA/DIF, Bruyeres-le-Chatel, France — Exhaustive studies have described the behaviour of materials and wave propagation across them when they obey to the Beth's first condition. This means that the equations of state and the isentropes in the (P,V) plane are convex and that the sound speed is an increasing function of the density. In that case, steady dynamic pressure waves are compression shock waves or expansion waves. But materials can often reach states where this condition is violated. This happens for instance with phase transitions, dissociations, near the critical point, and in BZT fluids. Across these thermodynamic states, wave propagation has been studied only in a few specific cases by Zel’ dovitch, Duvall, Plohr, Menikoff, Brun and their co-authors, but the general case remained to be explained. Our purpose is to provide the explanation of the successive waves which can occur in the general case when a wave propagates through a material with a non convex equation of state. We show that decrease of the sound speed introduced isentropic compression waves in the middle of shock waves and released shocks in the middle of expansion fans. After basic phenomena explanations, we illustrate them on the example of a virtual material which gathers all these cases. Hydrocode calculations based on this material show the difficulties of numerical schemes to reproduce the physical features.

11:15AM G4.00003 Isentropic Compression Studies of Energetic Composite Constituents

MELVIN BAER, CLINT HALL, MIKE HOBBES, Sandia National Laboratories, RICK GUSTAVSEN, DANIEL HOOKS, STEVE SHEFFIELD, Los Alamos National Laboratory — A series of quasi-isentropic magnetic pulse compression experiments using the Sandia Z accelerator and DICE small pulser have provided new insights in material behavior of the various constituents typically used in energetic composites. In this presentation, we overview a method used to determine appropriate constitutive and EOS property data using the combination of forward and backward procedures with optimization software. Sensitivity analysis is presented to assess the uncertainties of the experimental measurements and their effects in determining material response. These data interrogation techniques were applied at a ramp loading condition up to 50 Kbar over duration of ~500 ns in panel configurations containing explosive crystals (HMX and RDX), binders (Estone, Teflon, Kel F and HTBP) and composites (PBX9501, PBS9501, Al/Teflon).

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

11:30AM G4.00004 Wave propagation in materials with non convex equation of state

OLIVIER HEUZE, STEPHANE JAOUEN, HERVE JOURDREN, CEA/DIF, Bruyeres-le-Chatel, France — Exhaustive studies have described the behaviour of materials and wave propagation across them when they obey to the Beth's first condition. This means that the equations of state and the isentropes in the (P,V) plane are convex and that the sound speed is an increasing function of the density. In that case, steady dynamic pressure waves are compression shock waves or expansion waves. But materials can often reach states where this condition is violated. This happens for instance with phase transitions, dissociations, near the critical point, and in BZT fluids. Across these thermodynamic states, wave propagation has been studied only in a few specific cases by Zel’ dovitch, Duvall, Plohr, Menikoff, Brun and their co-authors, but the general case remained to be explained. Our purpose is to provide the explanation of the successive waves which can occur in the general case when a wave propagates through a material with a non convex equation of state. We show that decrease of the sound speed introduced isentropic compression waves in the middle of shock waves and released shocks in the middle of expansion fans. After basic phenomena explanations, we illustrate them on the example of a virtual material which gathers all these cases. Hydrocode calculations based on this material show the difficulties of numerical schemes to reproduce the physical features.

11:45AM G4.00005 Solitary and shock waves in discrete double power law materials

ERIC HERBOLD, VITALI NESTERENKO, Department of Mechanical and Aerospace Engineering, University of California at San Diego, La Jolla, California 92093-0418 — A novel strongly nonlinear metamaterial is composed using a periodic arrangement of toroidal rings between plates. The toroids are considered massless strongly nonlinear springs where the force versus displacement relationship is described by two additive power-law relationships. In these systems the nonlinearity is due to the dramatic change of the contact plane, which starts as an arbitrarily thin circle then increases in thickness with increasing compression. Solitary and shock waves are examined numerically and experimentally using three different types of polymer or rubber o-rings allowing mitigation of higher amplitude shock impulses in comparison with granular systems. In these systems a train of pulses can consist of two separate groups related to two strongly nonlinear regimes with different values of exponents, depending on the amplitude. In experiments two types of shock waves (monotonic or oscillatory) were observed depending on the type of o-rings.

1This work is supported by the NSF (Grant No. DCM03013220).

12:00PM G4.00006 Phase kinetics and Nonlinear Wave Propagation

ROGER MINICH, DANIEL ORLIKOWSKI, JEFFREY NGUYEN, LLNL, LLNL COLLABORATION — The properties of phase transitions in high pressure experiments are primarily inferred from velocity time histories. The recent development of the graded density impactor for tailoring pressure drives has provided information concerning phase transitions for thermodynamic paths different from a Hugoniot. The phase kinetics are encoded in the nonlinear wave propagation where dissipative and dispersive effects along with the nonlinear elastic response influence the shape of the wave. The observation of traveling wave structures suggests how to determine the relative contributions from the competing effects. A brief discussion of how the dissipation and dispersion in the nonlinear wave is related to a Langevin representation for the generation of new phase will be presented. Comparison to experimental data for Bi, Fe, and water will be shown.

12:15PM G4.00007 Improved EOS for describing high-temperature off-hugoniot states in epoxy

R.N. MULFORD, N.E. LANIER, D. SWIFT, J. WORKMAN, Los Alamos National Laboratory, PETER GRAHAM, ALASTAIR MOORE, Atomic Weapons Establishment, UK — Modeling of off-hugoniot states in an expanding interface subjected to a shock reveals the importance of a chemically complete description of the materials. Hydrodynamic experiments typically rely on pre-shot target characterization to predict how initial perturbations will affect the late-time hydrodynamic mixing. However, it is the condition of these perturbations at the time of shock arrival that dominates their eventual late-time evolution. In some cases these perturbations are heated prior to the arrival of the main shock. Correctly modeling how temperature and density gradients will develop in the pre-heated material requires an understanding of the equation-of-state. In the experiment modeled, an epoxy foam layered package was subjected to tin L-shell radiation, producing an expanding assembly at a well-defined temperature. This assembly was then subjected to a controlled shock, and the evolution of the epoxy-foam interface imaged with x-ray radiography. Modeling of the data with the hydrodynamics code RAGE is unsuccessful under certain shock conditions, unless condensation of chemical species from the plasma is explicitly included. The EOS code CHEETAH was used to prepare suitable EOS for input into the hydrodynamics modeling.

Tuesday, June 26, 2007 10:30AM - 12:30PM – Session G5 Equation of State II Fairmont Orchid Hotel Plaza III
10:30AM G5.00001 Multiphase equation of state and strength properties of beryllium from ab initio and quantum molecular dynamics calculations, GREGORY ROBERT, ARNAUD SOLLIER, CEA-DIF BP 12 91680 Bruyères le Chatel — In the framework of density functional theory, static properties and phonons spectra of beryllium have been calculated under high compression (for pressures up to four Mbar) for two solids phases: hexagonal compact (hcp) and body-centred cubic (bcc). The melting curve and some isotherms in the liquid phase are calculated using quantum molecular dynamic. The coupling of these theoretical data to a quasi-harmonic approach (Debye model) for these three phases (two solids and a liquid) allows us to suggest a new theoretical phase diagram as well as a multiphase equation of state in a large range of pressure and temperature. The resulting 300K isotherm and Hugoniot curves as well as the evolution of the shear modulus with both pressure and temperature are in good agreement with available data. The elastic constants calculated under shock loading allow us to fit the coefficients of constitutive laws at very high pressures and high strain rates.

10:45AM G5.00002 Hugoniot, shock melting and high pressure strength properties of beryllium1. MICHAEL DESJARLAIS, MARCUS KNUDSON, RAYMOND LEMKE, Sandia National Labs — The shock melting of beryllium has gained interest of late due to its potential as an ablative material in inertial confinement fusion capsules. Recently, experiments utilizing the flyer plate capability at the Sandia Z accelerator were performed to determine the Hugoniot and the shock melting properties of polycrystalline beryllium. Composite aluminum/copper flyer plates were used to shock load beryllium samples to pressures ranging from 1 to 4 Mbar. Multiple sample thicknesses allowed for the measurement of the release wave velocity, which is sensitive to the phase of the material in the shocked state. The release wave structure also provides estimates of material strength. Results of these experiments will be discussed and compared to detailed quantum molecular dynamic calculations which provide insight into the shock melting of beryllium and the extent of the coexistence region on the Hugoniot.

1 Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000

11:00AM G5.00003 Multiphase Equation of State of Carbon at Extreme Conditions, LORIN X. BENEDIT, ALFREDO A. CORREA, ERIC R. SCHWEGLER, DAVID A. YOUNG, Lawrence Livermore National Lab — We describe our scheme to construct a multiphase EOS model for carbon at high pressures and temperatures. Three phases are considered: diamond, BC8, and liquid. Ab initio calculations of cold curves and phonon densities of states, as well as direct QMD computations of EOS are used to constrain simple analytic models for the free energies of the individual phases. Special care was taken to extract the anharmonic terms in the solid phases, and to compute their effect on the Hugoniot and phase lines. We discuss the challenges associated with using this information, together with experimental results, to produce an EOS table for use in hydro-code applications.

11:15AM G5.00004 A new tabular EOS for hydrogen isotopes, DIDIER SAUMON, Los Alamos National Laboratory — The Saumon-Chabrier EOS model for hydrogen has been greatly improved, expanded to cover new physical regimes, and generalized to all three isotopes of hydrogen. The new table covers $1 \leq T \leq 10^9$K and $10^{-10} \leq \rho \leq 10^3$g/cm$^3$. At low temperatures, gaseous, liquid and solid molecular phases are included, as well as the monatomic solid plasma. The fluid phase is based on the chemical picture that describes interacting H$_2$, H, H$^+$ and electrons. Quantum corrections on the dense molecular, atomic and ionic fluids are included. The plasma model considers electron degeneracy, screening, relativistic effects, as well as strong plasma coupling. Interactions between charged and neutral particles have received particular attention as they control the pressure ionization of hydrogen. Notably, we found that previous predictions of a first order "plasma phase transition" based on this type of model are inherent to their construction and are not credible. This new model does not predict such a transition. A brief overview of the model will be followed by extensive comparisons with static and dynamic compression data and ab initio simulations.


11:45AM G5.00006 Sound Velocity in Shock-Compressed Samples and Equation of State of Tin1, K.V. KISHSCHENKO, V.E. FORTOV, I.V. LOMONOSOV, JIHT RAS, Moscow, Russia, M.V. ZHERNOKLETOV, A.E. KOVALEV, A.B. MEZHEVOV, M.A. MOCHALOV, M.G. NOVIKOV, A.N. SHUIKIN, RFNC-VNIIEF, Sarov, Russia — Equation of state for matter over a wide range of pressures and temperatures is required for simulations of processes in shock-compressed media. In the present study we have obtained data on the sound velocity behind the shock-wave front in tin at pressures $P \geq 77 \div 135$ GPa. We measure the shock and rarefaction overtake method with CCl$_4$ and CaF$_2$ as the analyzer liquids. We propose a semiempirical equation of state for tin with taking into account the polymorphs transformation, melting, and evaporation effects. Calculation results are compared with the newly acquired and available experimental data at high energy densities. The multi-phase equation of state obtained can be used efficiently in modeling of physical phenomena at high dynamic pressures.

1 This work was supported by RFBR, grant 06-02-17464

12:00PM G5.00007 Tabular Multiphase Equations of State for Metals and Their Applications, PAVEL LEVASHOV, KONSTANTIN KISHSCHENKO, JIHT RAS, Moscow, Russia — In this work we use multiphase equations of state in tabular form for numerical simulation of different problems of shock-wave physics. These equations of state take into account melting, evaporation and sublimation phase transitions and can be applied in metastable regions including those under negative pressure. We use two interpolation techniques for calculation of thermodynamic properties: (i) adaptation of a rectangular grid to phase and metastable boundaries and (ii) triangular grid in every region of phase diagram. Both techniques allow one to unambiguously determine the phase state of a given point of phase diagram. For very fast processes different temperatures for ions and electrons can be used. Several applications of multiphase equations of state were presented: simulation of the initial stage of electrical explosion of metal wires and foils, hypervelocity impact, interaction of intense laser pulses with matter etc. Information about phase state in every point of the flux allows us to study phase transition waves, apply different destruction criteria and analyze processes in metastable regions. The work is done under RFBR financial support, grant 06-02-17464.
propagation in PMMA and the RDX-based explosive PBX 9205, PETER WASHABAUGH, University of Michigan. Some preliminary 3D work will also be presented.

The bulk mechanical and chemical responses of explosives are largely determined by microstructures. Here we present some recent progress in grain-scale discrete element simulation of shock responses of granular explosives of Fluid Physics, China Academy of Engineering Physics, Mianyang, Sichuan 621900, China — The stress- and EOS. A kink was found on the measured Hugoniot curve. The EOS of the high-pressure phase will be discussed. MD simulation studies were also performed to discuss the mechanism of B1-B2 phase transition.

Tuesday, June 26, 2007 10:30AM - 12:30PM

10:30AM G6.00001 An initial investigation of the sub-microsecond features of dynamic crack propagation in PMMA and the RDX-based explosive PBX 9205, PETER WASHABAUGH, University of Michigan. LARRY HILL, Los Alamos National Laboratory — A dynamic crack propagating in a brittle material releases enough thermal energy to produce visible light. The mechanism of phase transition and equation of states (EOS) have been unknown. Hugoniot-measurement experiments were performed on RbCl single crystals by means of the inclined-mirror method combined with propellant guns to study the B1-B2 phase transition and EOS. Experiments were conducted in specimens to simulate an infinite plate for 20 μs. The initial specimens were 152 mm square by 6 mm thick acrylic sheets, and were fabricated to study non-steady near-wave-speed crack propagation. A variant of this specimen embedded a 25 mm x 3 mm PBX 9205 pellet to explore the influence of dynamic Mode-I cracks in these materials. The crack was initiated by up to 0.2 g of Detasheet placed along a precursor 50 mm long notch, with a shield to contain the reaction products and prevent propagation along the fractured surfaces. The crack was studied by means of a streak camera and a Fourier-filter of the light reflecting off the newly minted surfaces. The sub-microsecond behavior of holes initiating, preceding and coalescing with the main crack were observed in the PMMA samples. The embedding and mechanical loading of explosives by this technique did not initiate a self-sustaining reaction in preliminary testing.

10:45AM G6.00002 Brazilian disc testing of a UK PBX below the glass transition temperature.

11:00AM G6.00003 Recent Developments in Shear Ignition of Energetic Materials Using Hybrid Drop Weight-Hopkinson Bar, VASANT JOSHI, NSWC, Indian Head, Maryland — The sensitivity and mechanical behavior of energetic material is highly dependent on its constituents. Cast as well as cured (like PBX) types of explosives have mechanical properties significantly different from metals and the assumption of isotropy may not be valid beyond Strain of isotropy. While Split Hopkinson Pressure Bar (SHPB) can be successfully used to obtain mechanical properties of these soft explosives at strain rates up to 5,000/sec, ignition conditions are seldom achieved in SHPB tests. In very sensitive explosives, if ignition occurs in very small sample at extremely high strain rates, it would be very difficult to calculate the energy and energy rate that led to successful ignition. In contrast to the SHPB test, the drop-weight test, uses gravitational acceleration to impart a nearly constant velocity at the instant of impact. The Drop weight test is intended to obtain ignition, only as a go-no go condition, due to the variation of velocity, either due to change in the initial height or small changes in friction or drag. Due to lack of quantifiable parameters, the result from this test is not suitable for modeling, which is important in development of new explosive formulation. In order to overcome this barrier and allow evaluation of the susceptibility of the different formulations to ignition, a new test was recently developed. This test is called Hybrid Hopkinson Bar Drop Weight test, which overcomes shortcomings of two systems. When an explosive sample is compressed between two rigid flat surfaces and the material freely slides on the rigid plates without pinning, the mechanical energy is uniformly dissipated throughout the sample. In absence of any pressure gradient, pure-shear conditions apply throughout the sample. The ignition in this case, will not be localized at the edges, which is the basis for obtaining ignition condition in the new apparatus. Using this method, hydroxy-terminated polybutadiene (HTTP) bonded explosives, PBXN-110 and PBXW-128, cast TNT and Comp B are compared for their ignition thresholds. This method uses novel approach in diagnostics techniques, data acquisition and reduction methods to simultaneously quantify mechanical properties and ignition conditions.

11:30AM G6.00004 Pressure Dependence of Crack Growth and Plastic Flow Processes in Composite Plastic Bonded Explosives, DONALD WIEGAND, ARDEC, Picatinny ARSENAL, KEVIN ELLIS, AWE, UK — The stress-strain curves of composite plastic bonded explosives can be divided into two regions as a function of pressure. In a low pressure region stress as a function of increasing strain exhibits a maximum followed by work softening while in the higher pressure region yield followed by work hardening is observed. The results indicate that the work softening is due to crack growth damage and the work hardening is associated with plastic flow. In the low pressure region the compressive strength increases linearly with pressure and in the higher pressure region the flow stress (yield strength) increases approximately linearly with pressure but with a much lower slope. Therefore, the results indicate that in the low pressure region the stress required for plastic flow is higher than the stress for crack growth so crack processes dominate while in the higher pressure region the stress required for plastic flow is lower than the stress required for crack growth and so plastic flow dominates.

11:45AM G6.00005 Individual contributions of friction and impact on non-shock initiation of high explosives, PAUL PETERSON, GABE AVILUCEA, ROBERT BISHOP, JOHN SANCHEZ, LANL — Throughout the years a variety of tests have been designed which provide insight into the sensitivity of high explosives (HE) to non-shock initiation. Various standard tests such as the LNLN drop weight impact, LLNL drop hammer, drop tower and skid tests have been developed to measure energetic response of explosives subjected to a combination of friction and oblique impact. In addition, the BAM test (for HE powders on roughened ceramic) and ABL friction test (powders or solids on roughened metal) have been developed for testing HE under frictional loading. In an effort to understand first principles of non-shock initiation, we have designed a series of tests to try to isolate friction and impact during the inlet of HE. An initial series of tests have been completed with PETN, HMX, and as-pressed pellets of PBX 9501 (95 wt. percent HMX, 5 wt. percent inert binder), PBX 9502 (95 wt. percent TNT, 5 wt. percent inert binder), Cyclotol (75 wt. percent RDX/25 wt. percent TNT), and Comp B (60 wt. percent RDX, 40 wt. percent TNT). The results suggest that some types of high explosives are relatively insensitive to pure impact and pure friction but relatively sensitive to insults involving a combination of impact and friction.

12:00PM G6.00006 Grain Scale Discrete Element Simulation of Shock Responses of Explosives, WENQIANG WANG, JIDONG YU, HUA FU, CANGLI LIU, FENG ZHAO, CHENGWEI SUN, Laboratory for Shock Wave and Detonation Physics, Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang, Sichuan 621900, China — The bulk mechanical and chemical responses of explosives are largely determined by microstructures. Here we present some recent progress in grain-scale discrete element simulation of shock responses of granular explosives and PBXs. The discrete element models can be built based on Voronoi tessellation as well as real micrographs. Our studies have been focused on the damage and fracture issues and the evolution of hot spots. The results are roughly in agreement with those from mesh-based simulation techniques. We will discuss the newly developed discrete element force models. Some preliminary 3D work will also be presented.
Tuesday, June 26, 2007 10:30AM - 12:15PM — Session G7 Continuum and Multiscale Modeling I Fairmont Orchid Hotel Promenade III

10:30AM G7.00001 A Two-Scale FEM formulation for Heterogeneous Materials, ANXITE IONITA, ERIC MAS, BRADFORD CLEMENTS, Los Alamos National Laboratory, Theoretical Division — We present a new Two-Scale Finite Element formulation, in the dynamic case, for the heterogeneous materials (for example, high explosives and other composites). The method employs two sets of finite element discretizations: one global (associated with the $1^{st}$ scale) and, for each element in the mesh at the $1^{st}$ scale, a local discretization (associated with the $\Pi^{nd}$ scale). Using the principle of virtual work in conjunction with the localization problem the Two-Scale FEM equations are established for two cases: the case when the representative volume element (RVE) is much smaller than the finite element size of the $1^{st}$ scale, and for the case when the RVE size become comparable with the finite element of the $1^{st}$ scale. The obtained equations are decoupled in the sense that the dynamics equations are solved relative to the $1^{st}$ scale while the $\Pi^{nd}$ scale is used to determine the material response. The proposed approach allows more flexible and a better correlation with experiments and eventually can be incorporated in a larger context analysis involving heterogeneous materials. Numerical examples are included. LA-UR-06-5889.

10:45AM G7.00002 Multiscale Modeling of Plastic Bonded Explosives, GRANT SMITH, DMITRY BEDROV, University of Utah, OLEG BORODIN — We have developed a multiscale modeling paradigm for the prediction of the viscoelastic properties, equation of state and yielding behavior of plastic bonded explosives (PBXs). In our multiscale modeling approach the components of the explosive (e.g., energetic material, metal and binder) are explicitly resolved and the material point method (MPM) is utilized to predict the response of the composite material to loading (isentropic, shock, etc.). This data are then utilized to develop equation-of-state and constitutive models for the PBX. The properties of the components are determined either from atomistic simulations or are taken from the literature. Force fields for the atomistic simulations in turn have been developed based upon high-level electronic structure calculations of model compounds and molecular complexes. Hence, our multiscale simulation approach systematically bridges length scales from atomistic to macroscopic. Applications of this approach to PBX-9501 and other PBXs will be considered.

11:00AM G7.00003 Modeling the Asymmetric Burning of Agglomerate Particles, CLINTON RICHMOND — A model has been developed to describe asymmetric burning effects due to oxide caps or other substances on the surface of agglomerate particles. The model accounts for the burning behavior of single particles when they are combined together in an agglomerate of particles. The model calculates the available surface area that is exposed to burning by the geometric formation of the agglomerate of the combining particles. Analyzing analytic techniques are applied to the burning behavior of the agglomerate of particles so that its burning effects can be compared to the burning effects from the uncombined, single particles.

11:15AM G7.00004 Modelling of detonation in PBX 9502 with a stiffened-gas EOS mixture model, CHARLES KIYANDA, MARK SHORT, Los Alamos National Laboratory — An analytically tractable model of detonation in PBX 9502 is developed. It consists of a mixture of reactant and product materials, with each component represented by a stiffened-gas equation of state. The five free thermodynamic parameters in the model allow us to address some of the restrictions of simpler analytical models. We first explore generic properties of the steady 2D detonation structure under this model. Secondly, we show that fitting of the thermodynamic data to experimental data on reactant and product properties yields non-intersecting Hugoniot curves. The associated chemical kinetic scheme consists of two reaction steps. The first step has a pressure dependent rate term. It takes the reactants to an intermediate state, a mixture of effectively mostly gaseous products with some solid carbon. The second step models the clustering of solid carbon atoms. Pop-plot and detonation velocity vs. curvature data are used to fit the chemical kinetic parameters. Finally, the linear stability of PBX 9502 detonation waves modeled by the stiffened gas system is studied.

11:30AM G7.00005 Metal Particle Heating and Acceleration in Condensed Explosives, ROBERT RIPLEY, Martec Limited, FAN ZHANG, DRDC Suffield, FUE-SANG LIEN, University of Waterloo — For condensed explosives containing metal particle additives, a characteristic parameter relating the detonation reaction zone length ($L_r$) to the particle size ($d_p$) can be defined as $\delta = d_p/L_r$. The detonation reaction zone length is typically $0.01 < L_r < 100$ mm, whereas metal particle sizes of $100$ nm $< d_p < 1$ mm can be employed. This indicates a potential range of $10^{-6} < \delta < 10^2$. The limiting case of $\delta \ll 1$ involves frozen shock/particle interaction; for $\delta >> 1$ the interaction consists of a thin-detonation-front diffraction followed by expanding products flow. The intermediate case of $\delta \approx 1$ has been studied previously as a function of metal mass fraction and particle packing to determine momentum and heat transfer during the detonation interaction time. Results indicate a strong dependence of particle acceleration and heating rate on $\delta$ for high metal mass fraction conditions. The present study employs 3D mesoscale simulation to further conduct parametric studies in the $0.1 \le \delta \le 10$ range by varying the particle diameter, particle metal and explosive material. The results are quantified to determine macroscopic physical models for particle acceleration and heating.

11:45AM G7.00006 Rate-Independent Material Model to Describe the Shock and Ramp Wave Loading Response of 6061-T6 Aluminum to 22 GPa, J.M. WINEY, W. MAMUN, Y.M. GUPTA, Wash. State Univ. — A rate-independent phenomenological material model has been developed to describe the response of 6061-T6 aluminum for shock loading to 22 GPa and ramp wave loading to 4 GPa. To describe the mean stress response of the material, existing isothermal pressure-volume data from hydrostatic compression experiments were utilized. The elastic shear response was modeled by assuming that Poisson’s ratio is constant. Material strength was described using a von Mises yield surface, together with nonlinear strain-hardening. Simulations using this material model were performed to compare with experimental wave profile data for shock and ramp wave loading. Our simulations show better agreement with the experimental results compared to previous materials models. In particular, experimental features such as the speed of the plastic wave, the ramping behavior between the elastic and plastic waves, and the speed of the release wave from the shocked state are described well by our model. Work supported by DOE.
12:00PM G7.00007 Nickel based superalloy containment case design: constitutive modeling and computational analysis. ANDREW RUGGIERO, NICOLA BONORA, GIOVANNI TORRICE, University of Cassino, MARCO DI SCIULVA, MARCO DEGIANNINI, MASSIMILIANO MATTONE, MARCO GHERLONE, Polytechnics of Turin, CARLO FROLA, Avidiopop S.p.A. — Quasi-static and dynamic characterization of nickel based superalloy Waspaloy® has been performed at the University of Cassino. Quasy-static tensile tests have been carried out on both round bar specimens, to obtain the flow stress curve at low strain rates, and hourglass specimens, to investigate damage evolution with plastic strain. The mechanical behavior at high strain rates has been obtained by means of a direct tension split Hopkinson Bar, which allows the characterization of the material via the CTH code. Experimental results show that the flow stress increases, the failure strain increases while the yield strength decreases, in some intervals of the range considered. This singular behavior has been modeled and implemented in a Finite Element Method commercial code in order to perform numerical simulations of experimental ballistic tests carried out at the Polytechnics of Turin, using an airgun facility. Good agreement has been found between FEM simulations and experimental results.

Tuesday, June 26, 2007 1:45PM - 3:15PM — Fairmont Orchid Hotel Amphitheater

1:45PM H2.00001 Nonmetal-to-metal transition in warm dense hydrogen and helium1. RONALD REDMER, BASTIAN HOLST, ANDRE KIETZMANN, NADINE NETTELMANN, Institute of Physics, University of Rostock, D-18051 Rostock, MICHAEL P. DESJARLAIS, THOMAS R. MATTSSON, Pulsed Power Sciences Center, Sandia National Laboratories — The precise knowledge of the equation of state of hydrogen and helium, especially at extreme conditions of pressure and temperature, is not only of fundamental interest but also necessary for models of interiors of giant planets such as Jupiter and Saturn. We have performed ab-initio quantum molecular dynamics (QMD) simulations for dense hydrogen and helium to study the thermophysical properties and the nonmetal-to-metal transition at high pressures. We present new results for the equation of state and the Hugoniot curves in the warm dense matter region. The optical conductivity is calculated via the Kubo-Greenwood formula from which the dc conductivity as well as the reflectivity are derived. We compare our results with shock wave experimental data as well as with other theoretical approaches. As a further application and test of the QMD equation of state data, the interiors of Jupiter and Saturn are modelled by solving the hydrostatic equation within a three-layer model.

1 This work was supported by the Deutsche Forschungsgemeinschaft within the SFB 652.

2:00PM H2.00002 Density Functional Theory in High Energy Density Physics: phase-diagram and electrical conductivity of water. THOMAS R. MATTSSON, Sandia National Laboratories — Atomic simulations employing Density Functional Theory (DFT) have recently emerged as a powerful way of increasing our understanding of materials and processes in high energy density physics. Knowledge of the properties of water (equation of state, electrical conductivity, diffusion, low-energy opacity) is essential for correctly describing the physics of giant planets as well as shock waves in water. Although a qualitative picture of water electrical conductivity has emerged, the necessary quantitative information is scarce over a wide range of temperature and density. Since experiments can only access certain areas of phase space, and often require modeling as a part of the analysis, Quantum Molecular Dynamics simulations play a vital role. Using finite-temperature density functional theory (FT-DFT), we have investigated the structure and electronic conductivity of water across three phase transitions (molecular liquid/ionic liquid/supersonic electronic liquid). The ionic contribution to the conduction is calculated from proton diffusion and the electronic contribution is calculated using the Kubo-Greenwood formula. The calculations are performed with VASP, a plane-wave pseudo-potential code. There is a rapid transition to ionic conduction at 2000 K and 2 g/cm³, whereas electronic conduction dominates at temperatures at and above 6000 K[1]. Contrary to earlier results using the Car-Parrinello method[2], we predict that the fluid bordering the superionic phase is conducting above 4000 K and 100 GPa. Our comprehensive use of FT-DFT explains the new findings. The calculated conductivity is compared to experimental data.

I gratefully acknowledge Mike Desjarlais, my collaborator in this effort. The LDRD office at Sandia supported this work. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.


2:30PM H2.00003 The relation between solitons and interactions in bcc materials. JOHANNES ROTH, ITAP, University of Stuttgart — Shock waves in simple crystal structures are frequently accompanied by solitons, at least in molecular dynamics simulations. In this paper results for the case of bcc-materials shocked along a three-fold axis are reported. Pair potentials and generalized EAM potentials are studied. The influence of the Cauchy pressure in contrast to EAM. For this type of interaction the solitons are strongly depressed for negative Cauchy pressures. For the Dzugutov potential the influence of the Cauchy pressure is investigated by comparing iron and chromium. Solitons are observed for all interactions, but their strength and velocity vary. A modification of the Zhou-Wadley two- and three-body potential [Comp. Mat. Sci., in press] is introduced which permits a controlled variation of the Cauchy pressure in contrast to EAM. For this type of interaction the solitons are strongly depressed for negative Cauchy pressures. For the Dzugutov potential [PRB 72 (2005) 14126] a close relation between a subsonic phase transition into an ω-phase and supersonic solitons has been observed. A similar relation has not been found for iron and other interactions, although it might be favorable energetically. By ab-initio calculations with VASP it is shown that the ω-phase transition in iron is surpassed by the transition into the hcp-phase.

2:45PM H2.00004 Ab initio Molecular Dynamics Simulations of Water Under Shock Conditions1. N. GOLDMAN, LLNL, C.J. MUNDY, Pacific Northwest Natl. Lab, I-F. W. KUO, E.J. REED, L.E. FRIED, LLNL, A. CURIONI, IBM Research, Zurich Research Lab — We report herein first principles simulations of water undergoing shock loading of velocities from 5 – 11 km/s. Shocked aqueous solutions are of particular interest to earth and planetary sciences, and the chemical reactivity that occurs within such hot, compressed systems. The Multi-Scale Shock Method (MSSM) uses a Lagrangian-derived constraint dynamics to restrict a molecular dynamics simulation to the thermodynamic states found in the shock. This allows for simulations with much smaller system sizes than previously required, and for significantly longer time scales than previously achievable. Consequently, for the first time, we have been able to conduct quantum simulations of a shocked material. We show that Density Functional Theory (DFT) molecular dynamics results compare extremely well to experiments on the water shock Hugoniot. We also present results for the ionic conductivity as well as the concentrations and lifetimes of chemical species found therein. Our results represent the strongest confirmation of the accuracy of DFT at high pressure and temperature that we know of, to date.

1This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.
Aluminum oxynitride (AlON) is a transparent, polycrystalline cubic spinel. The results of investigations show that at significantly high densities the fraction of bound states diminishes, and a crystallization can occur in the simulation box. This phenomenon exists at relatively low temperatures in the limited range of densities and at heavy-light particle mass ratio higher than 80 in 3D case. The crystal consists of heavy particles on the background of highly degenerate light particles; at certain conditions the heavy particle can form antiferromagnetic crystal-like structure. The crystal melts at temperature increase (the Lindemann criterion is valid in this case) and heavy-light particle mass ratio decrease (quantum melting). Our simulations generalize the earlier results for one-component plasma and can be applied to a number of problems: semiconductors under pressure, Coulomb crystals in white dwarfs and neutron stars, ion crystals in traps etc. Coulomb crystallization is also considered to be related to the high-temperature superconductivity. This work is supported by the CRDF and the Ministry of Education of Russian Federation Grant No. Y2-P-11-02.

In a recent series of papers, we have made a study of the shock response of a number of polymers, whilst systematically changing their structure, for example side group size (polyethylene, polypropylene and polystyrene) or replacement of hydrogen atoms (polyethylene, polyvinylidene difluoride and polytetrafluoroethylene). In this study, we examine a single polymer, polyethylene in two structural forms – high molecular weight and cross-linked. In this study, we examine a single polymer, polyethylene in two structural forms – high molecular weight and cross-linked. The crystal consists of heavy particles on the background of highly degenerate light particles; at certain conditions the heavy particle can form antiferromagnetic crystal-like structure. The crystal melts at temperature increase (the Lindemann criterion is valid in this case) and heavy-light particle mass ratio decrease (quantum melting). Our simulations generalize the earlier results for one-component plasma and can be applied to a number of problems: semiconductors under pressure, Coulomb crystals in white dwarfs and neutron stars, ion crystals in traps etc. Coulomb crystallization is also considered to be related to the high-temperature superconductivity. This work is supported by the CRDF and the Ministry of Education of Russian Federation Grant No. Y2-P-11-02.

### Session H3 Stress-Strength Measurements I

#### 1:45PM H3.00001 Phenomenological viscous-elastic-plastic model of dynamic yield of Cu

**OLGA IGNATOVA, RFNC-VNIIEF** — Taken together, the fundamental mechanisms that govern material flow under conditions of intensive loading comprise a multifaceted set, with each facet possessing its own domain of influence. These mechanisms include dislocation multiplication, grain size modification, twinning, and the formation of periodic shear bands during high-rate deformation. Existing flow stress models do not possess the capability of accounting for all of these mechanisms. Existing models are, for the most part, empirical. Those which attempt to account for the fundamental mechanisms responsible for material flow tend to be based on dislocation mechanics. Some include a number of internal state variables to try to account for history-dependent changes in morphology. None accounts for the full complexity of material behavior. An observation that can be made of existing models is that the greater the number of physical mechanisms accounted for, the greater the number of empirical parameters. In this work we present a new phenomenological elastic-viscoplastic flow stress model for M1 copper that accounts for variations in grain size, and does so with a reasonably small set of empirical parameters.

#### 2:00PM H3.00002 Application of Lagrangian Analysis to the Unloading Velocity-Time Signals of Flyer-Plate Experiments

**JAMES STOLKEN, MUKUL KUMAR, JEFFREY NGUYEN, REED PATTERSON, Lawrence Livermore National Laboratory** — Lagrangian analysis (LA) has been applied to a broad range of dynamic solid-state experiments over the last forty years to infer material constitutive behavior under complex loading conditions and provides the analytical foundation to interpret current state-of-the-art experiments probing both the Equation-of-State and Deformation properties of materials. Using a combination of high-resolution computer hydro-code simulations and gas-gun driven flyer-plate experimental data, a new method of LA is developed that combines the two methods due to D.C. Wallace and P.J. Chen to infer the normal stress and strain response of the material just prior to unloading. This new method of LA is applied to infer the stress-strain response of copper samples of varying grain size. In the case of ductile metals, the results suggest an alternate interpretation of the “elastic” unloading response on release as a “plastic” reloading wave produced as the result of an elastic transition from compressive to tensile loading. Extensions to “re-shock” experiments and the development of three-stepped targets to explore the nature of the “plastic” reloading waves are discussed. This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

#### 2:15PM H3.00003 Longitudinal and Lateral Stress Measurements in Stainless Steel 304 Under 1D Shock Loading

**G. WHITEMAN, J.C.F. MILLETT, R.E. WINTER, AWE, Aldermaston, Reading, RG7 4PR, UK** — Interest in the behaviour of the common stainless steel grade 304 at high rates of strain is always high due to the materials regular use in industry. Longitudinal and lateral stresses during the shock loading of stainless steel 304 have been measured using manganin stress gauges. The shear strength has been shown to increase with impact stress. Comparison with a pure fcc metal (nickel) shows a significant increase in strength. Strengths are similar to those of mild steel, but the rate of increase with impact stress is much greater in SS304. These results are discussed in terms of structure and degree of alloying.

#### 2:30PM H3.00004 Shear Strength of Aluminum Oxynitride

**DATTATRAYA P. DANDEKAR, US Army Research Laboratory, Aberdeen Proving Ground, MD 21005, BRIAN A. M. VAUGHN, WILLIAM G. PROUD, PCS, Cavendish Laboratory, Madingley Road, Cambridge, CB3 0HE, UK** — Aluminum oxynitride (AlON) is a transparent, polycrystalline cubic spinel. The results of investigations on shock response of AlON permit determination of the equation of state, and shear strength retained under shock compression. Whereas the values of the HEL of AlON holds no surprises, the inelastic response of AlON reported in Ref. 1-4 differ significantly and is stress dependent. The results of Ref. 1-2 show that AlON retains a shear strength of 3 to 4 GPa when shocked up to around 20 GPa, but the results of Ref. 3-4 seem to suggest a possible loss of shear strength when shocked to 16 GPa and beyond. Our analysis examines the observed differences in the inelastic response of AlON reported in these four studies. 1. J. U. Cazamias, et. al., in Fundamental Issues and Applications of Shock-Wave and High Strain Rate Phenomena, Eds. Staudhammer, Murr, and Meyers, Elsevier, NY, 173 (2001). 2. B. A. M. Vaughn, et.al., Shock Physics, Cavendish Laboratory, Report SP/1092 (2001) 3. T. Sekine, et.al., J. Appl. Phys. 94, 4803 (2003). 4. T. F. Thornhill, et.al., Shock Compression of Matter-2005, Eds. Furnish, Eler, Russell, White, AIP, NY, 143 (2006).

#### 2:45PM H3.00005 Shear strength and HEL’s for various geological materials

**C.H. BRAITHWAITE, W.G. PROUD, J.E. FIELD, Cavendish Laboratory, Cambridge University, A.R. GUEST, De Beers Group Services** — Previous investigations (Braithwaite, Proud and Field: SCCM 2005, pp1435-1438) into geological materials have shown that for some materials no change in slope is seen in the Hugoniot curve up to 10 GPa (depending on the rock type). These shock pressures are well above the expected elastic limits of the materials. There is some hysteresis seen in release curves above a certain stress level. By using the plate impact facility it was possible to measure the shear strength of the materials and determine region of the HEL. It is shown that the start of hysteretic behaviour in the release paths does not correspond to the HEL.

#### 3:00PM H3.00006 Shear strength and its variation according to structure in shock-loaded polyethylene

**JEREMY MILLETT, AWE, Aldermaston, NEIL BOURNE, University of Manchester, ERIC BROWN, GEORGE GRAY, Los Alamos National Laboratory** — In a recent series of papers, we have made a study of the shock response of a number of polymers, whilst systematically changing their structure, for example side group size (polyethylene, polypropylene and poly styrene) or replacement of hydrogen atoms (polyethylene, polyvinylidene difluoride and polytetrafluoroethylene). In this study, we examine a single polymer, polyethylene in two structural forms – high molecular weight and cross-linked. In particular, the shock induced shear strength is determined, and the effects of structural variation noted.

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**Tuesday, June 26, 2007 1:45PM - 3:15PM**

**Session H3 Stress-Strength Measurements I**

**Fairmont Orchid Hotel Plaza I**

**Session H4 Experimental Developments III**

**Fairmont Orchid Hotel Plaza II**
1:45PM H4.00001 New Capabilities of 800 MeV Proton Radiography at Los Alamos. CYNTHIA SCHWARTZ, Los Alamos National Laboratory — Three new capabilities have recently been commissioned at the proton radiography facility at Los Alamos. A powder gun driver system has been installed and commissioned and a series of demonstration measurements have been completed. This powder gun is now regularly used to drive dynamic experiments. A new CMOS hybrid camera technology has been developed and fielded resulting in dramatic improvements in quantum efficiency as well as providing eight additional radiographic images per dynamic event. A proton x3 magnifier was designed, built and commissioned to provide improved radiographic resolution for 800 MeV proton radiography experiments. Details of these new capabilities will be presented along with data from recent experiments which utilized these new capabilities.

2:00PM H4.00002 Proton Radiography of a Thermal Explosion in PBX 9501. LAURA SMILOWITZ, BRYAN HENSON, JERRY ROMERO, Chemistry Division, LANL, BLAINE ASAY, MARY SANDSTROM, DE Division, LANL, PRAD COLLABORATION — The understanding of thermal explosions and burn propagation lags that of detonations and shock propagation. Diagnostics such as high energy radiography have been used to image shocks, but have been previously precluded from use in thermal explosions due to their stringent timing requirements: shock propagation can be synchronized to an external diagnostic while thermal explosion can not. This issue is solved by following the evolution of the ignition volume in a thermal explosion and using a laser pulse to provide a temperature jump in that central volume during the final thermal runaway leading to ignition. Details of the laser heating which minimize the perturbation of the thermal explosion will be discussed with comparisons between auto-ignited and laser ignited tests. Thermal explosion experiments have been conducted at the Los Alamos Proton Radiography facility and have yielded images of the evolution of ignition, post-ignition burn propagation, and case failure in a radially confined cylinder of PBX 9501.

2:15PM H4.00003 Direct Shock-Density Measurements using Plate Impact and Proton Radiography. PAULO RIGG, Los Alamos National Laboratory — Proton radiography (pRad) is a powerful new diagnostic with the potential of producing accurate (1%) direct density measurements from dynamically loaded materials. Experiments have been performed to investigate the feasibility of using proton radiography (pRad) to produce dynamic radiographs of shock-compressed materials during plate impact experiments. This work has involved the design, manufacturing, and testing of a new 40mm single-stage, powder driven gun. The development of methods to synchronize the shock event generated with the gun to proton output, and initial proof-of-principle experiments in Area C at LANSCE. To date, four symmetric impact experiments on aluminum and copper have been performed with successful synchronization. The method used to obtain synchronization of the shock event to proton beam output will be discussed and the results of our initial experiments will be presented.

2:45PM H4.00004 Neutron Resonance Spectrometry Shock Temperatures in Molybdenum. DAMIAN SWIFT, ACHIM SEIFTER, DAVID HOLTKAMP, VINCENT YUAN, DAVID CLARK, WILLIAM BUTTLER, Los Alamos National Laboratory — Neutron resonance spectrometry (NRS) has been used to measure the temperature in Mo during shock loading, giving temperatures higher than expected. The effect of plastic flow and non-ideal projectile behavior were assessed. Plastic flow was estimated to contribute a temperature rise of 55K compared with hydrodynamic flow, and 100-150K on release, consistent with pyrometry measurements. Simulations were performed of the HE flyer system used to induce the shock in the Mo sample. The simulations predicted that the flyer was slightly curved on impact. The resulting spatial variations in load, including radial components of velocity, were predicted to increase the apparent NRS temperature by 160K. These corrections are sufficient to reconcile the apparent temperatures deduced using NRS with the accepted properties of Mo.

3:00PM H4.00005 Detonation Shock Radius Experiments. DAVID LAMBERT, Air Force Research Laboratory/Munitions Directorate, JOSHUA DEBES, Air Force Research Laboratory, SCOTT STEWART, SUNHEE YOO, University of Illinois, Urbana-Champaign — A previous passover experiment [1] was designed to create a complex detonation transient used in validating a reduced, asymptotically derived description of detonation shock dynamics (DSD). An underlying question remained on determining the location of the initial detonation shock radius to start the DSD simulation with respect to the dynamical response of the initiation system coupling’s to the main charge. This paper concentrates on determining the initial shock radius required of such DSD governed problems. ‘Cut-back’ experiments of PBX-9501 were conducted using an initiation system that sought to optimize the transferred detonation to the desired constant radius, hemispherical shape. Streak camera techniques captured the breakout on three of the prism’s surfaces for the initial shock radius required of such DSD governed problems. The understanding of thermal explosions and burn propagation lags that of detonations and shock propagation. Diagnostics such as high energy radiography have been used to image shocks, but have been previously precluded from use in thermal explosions due to their stringent timing requirements: shock propagation can be synchronized to an external diagnostic while thermal explosion can not. This issue is solved by following the evolution of the ignition volume in a thermal explosion and using a laser pulse to provide a temperature jump in that central volume during the final thermal runaway leading to ignition. Details of the laser heating which minimize the perturbation of the thermal explosion will be discussed with comparisons between auto-ignited and laser ignited experiments. Thermal explosion experiments have been conducted at the Los Alamos Proton Radiography facility and have yielded images of the evolution of ignition, post-ignition burn propagation, and case failure in a radially confined cylinder of PBX 9501.

1:45PM H5.00001 A Geometry for Sub-Nanosecond X-Ray Diffraction from Laser-Shocked Polycrystalline Foils. JUSTIN WARK, ANDREW HIGGINBOTHAM, GILES KIMMINAU, WILLIAM MURPHY, BOB NAGLER, THOMAS WHITCHESTER, University of Oxford, UK, JAMES HAWRELIAK, DAN KALANTAR, HECTOR LORENZANA, BRUCE REMINGTON, LLNL, HUW DAVIES, LEE THORNTON, NIGEL PARK, AWE, Aldermaston, UK, STAN LUKEZIC, Pyramid St, Livermore, CA — In situ picosecond X-ray diffraction has proved to be a useful tool in furthering our understanding of the response of shocked crystals at the lattice level. To date the vast majority of this work has used single crystals as the shocked samples, owing to their diffraction efficiency, although the study of the response of polycrystalline samples is clearly of interest for many applications. We present here the results of experiments to develop sub-nanosecond powder/polycrystalline diffraction using a cylindrical pinhole camera. By allowing the incident X-ray beam to impinge on the sample at non-normal angles, the response of grains making a variety of angles to the shock propagation direction can potentially be interrogated.

1:45PM H5.00001 A Geometry for Sub-Nanosecond X-Ray Diffraction from Laser-Shocked Polycrystalline FoilsJW and BN are supported the EU Marie-Curie RTN ‘FLASH’
2:00PM H5.00002 High pressure X-ray diffraction studies on Bi$_2$-Sb$_2$Te$_3$ (x=0,1,2) materials. M. JACOBSEN, R. KUMAR, A. CORNELIUS, University of Nevada, Las Vegas — Recent Bi$_2$Te$_3$ based thermoelectric materials have gained importance due to their high thermoelectric figure of merit in thin films [3]. Pressure tuning of the thermoelectric figure of merit has been reported for several materials [1,2]. In order to investigate the bulk properties of Bi$_2$Te$_3$, Sb$_2$Te$_3$, and their solid solution in detail, we have performed structural studies up to 20 GPa. Our diffraction results show that all three compounds transform from the ambient pressure structure to a high pressure phase between 5 and 7 GPa. Details of the results will be discussed in this presentation. [1] Chen, G., Dresselhaus, M.S., Dresselhaus, G., Fleurlis, J.-P., and Caillet, T. Recent developments in thermoelectric materials. International Materials Reviews, 48, 45-66 (2003). [2] Rowe, D.M. CRC Handbook of Thermoelectric Materials. CRC Press, 1995. [3] Venkataramanu, R., Silvola, E., Colipdt, T., and O’Quinn, B. Thin-film thermoelectric devices with high room-temperature figures of merit. Nature, 413, 597-602, 2001.

1 Work at UNLV is supported by DOE EPSCoR-State/National Laboratory Partnership Award DE-FG02-00ER45835 and DOE Cooperative Agreement DE-FG08-98NV1341. Additional support for this project was provided by the UNLV Graduate Student Association.

2:15PM H5.00003 Static High Pressure X-ray Diffraction of Ti-6Al-4V. G. CHESNUT, N. VELISAVLJEVIC, L. SANCHEZ, Los Alamos National Lab — Ti-6Al-4V was examined under static-high pressure conditions using a diamond anvil cell. The angle-dispersive x-ray diffraction experiments were performed at the Advanced Photon Source, Argonne National Laboratory. Radial and axial geometry were used to examine multiple samples. The purpose of the experiment was to generate pressure-volume data at room temperature (which is non-existent in literature) and to examine deviatoric stress effects on such a hard alloy.

1 Supported by the US DOE under contract DE-AC52-06NA25396.

2:30PM H5.00004 Radiation-induced damage studies of energetic materials. M. PRAVICA, H. GIEFERS, Z. QUINE, D. ROMANO, D. YULGA, H. LIEMANN, HiPSEC, University of Nevada, Las Vegas, W. YANG, H. HOOKS, Los Alamos National Laboratory — We present studies of synchrotron radiation-induced decomposition of PETN and TATB under conditions of high pressure, high temperature, and crystalline orientation. We have found that the decomposition rate varies dramatically under all three of these variables. The experiments were performed using white beam synchrotron radiation at the 16 BM-B and 16 BM-D sectors of the HP-CAT beamline at the Advanced Photon Source. Diffraction line intensities were measured as a function of time using energy-dispersive methods and angular-dispersive methods TATB showed dramatic slowing of the decomposition rate with pressure implying a positive activation volume of the activated complex whereas PETN showed little change in decomposition rate with pressure. Increased temperature increased the radiation-induced decomposition rate of TATB. Finally, we found dramatic differences in the radiation-induced decomposition rate for single crystals of explosives depending upon their orientation relative to the polarized x-ray beam.

Tuesday, June 26, 2007 1:45PM - 3:15PM –
Session H7 Reactive Materials I — Fairmont Orchid Hotel Promenade III

1:45PM H7.00001 Reactive Nanolaminates as Model Materials for Controlling Initiation Thresholds under Shock and Electrical Loading, T. WEIHS, Johns Hopkins University — Over the last ten years a group of researchers at Johns Hopkins University have demonstrated the ability to control and predict the initiation and energy of exothermic reactions that self-propagate in foils with nanoscale layering. These exothermic reactions can be ignited with mechanical, electrical, optical or thermal pulses of energy and provide model materials for systemically varying and predicting initiation thresholds. This presentation will describe our efforts to quantify and predict how the initiation and propagation of these reactions depend on the nanoscale spacing of the reactants and their heats of reaction for mechanical and electrical loadings. Studies of mechanical deformation will also be presented. The free-standing foils or sheets are fabricated using vapor or mechanical processing methods and range in total thickness from 10µm to 1000µm. The individual layers within the foils range in thickness from 10nm to 10,000nm. Rod and plate geometries can also be fabricated. A common chemistry for formation reactions includes Ni and Al while a typical chemistry for a reduction/oxidation reaction would include Al and CuO. The reactants and their spacing are chosen to enable exothermic reactions that self-propagate at velocities ranging from 0.1 to 10m/s with maximum temperatures above 1000°C. Using mechanical impact tests and electrical discharge experiments we have measured thresholds for initiating reactions in these foils, and we have shown that the thresholds increase significantly with reactant spacing and with pre-mixing between the reactants. These measurements are compared with numerical predictions and show strong agreement. The mechanisms controlling the initiation of the reactions will be reviewed and the metastable phases that appear within the self-propagating reactions will be identified using in situ XRD experiments. Lastly, the strength of these materials will be characterized as a function of reactant spacing using standard tension tests.

2:15PM H7.00002 Investigation of Formulations Containing Perfluoro-Coated Oxide-Free Nano-Aluminum, A. WARREN, G. LAWRENCE, R. JOUET, Naval Surface Warfare Center, Indian Head Division — Plastic Bonded Explosive (PBX) samples were formulated incorporating oxygen-free nano-aluminum (nano-Al) that is passivated with a fluorinated carboxylic acid. This project investigated explosive formulations containing this coated nano-Al (C14/nanoAl). Small-Scale Shock Reactivity and Internal Blast Tests (SSSBT) determined the contribution of the C14/nanoAl in the early stages of the reaction. These results show that the volume of the dent of samples containing C14/nanoAl is twice as great as the dent volume of standard formulations, suggesting faster aluminum combustion than conventional Al formulations.

1 Funding provided by the US Navy IAR program.

2:30PM H7.00003 Preparation and Shock Reactivity Analysis of Novel Perfluoroalkyl-Coated Aluminum Nanocomposites, J.R. JOUET, J.R. CARNEY, J.M. LIGHTSTONE, A.D. WARREN, HIDIV, Naval Surface Warfare Center — The barrier to realization of the energy potential of metals is the comparatively slow rate of oxidation. The rate of oxidation is governed by diffusion of the fuel and oxidizer species. For Al, the Al$_2$O$_3$ surface oxide further slows this process. Replacement of this layer with organic molecules containing oxidizer species should result in a material that reacts fast enough to enable the energy release to contribute to explosives detonation. Passivation of unpassivated, oxide-free Al nanoparticles using C$_{13}$(F$_2$)$_x$CO$_2$H and C$_{15}$(F$_2$)$_x$CO$_2$H forming self assembled monolayers (SAMs) is reported with materials containing as much as 33 % Al. The fast reaction capability of the SAM-passivated material was investigated using time-resolved emission measurements of laser ablation experiments. Laser ablation can transfer momentum to a surface, since the ablated material applies a pulse of high pressure to the surface underneath it as it expands. Time-resolved emission results of the SAM-passivated materials were compared with oxide passivated Al nanoparticles coated with the same acids, C$_{13}$(F$_2$)$_x$CO$_2$H and C$_{15}$(F$_2$)$_x$CO$_2$H.
of information between QM and classical MD. Semi-empirical potentials, or in generating QM data for fitting their parameters, will share some comments. The time is ripe for new paradigms in the exchange of information under extreme conditions. As a result, one can legitimately worry about the quality of MD simulations in such regimes. Modern computational capabilities have made it possible to simulate very large systems at high pressures and temperatures. For example, the folding of proteins at high pressures and temperatures has been studied using MD simulations. These results indicate that the transition from floppy to rigid states is possible at high pressures and temperatures.

Dynamics Calculations Under Extreme Conditions

4:30PM J2.00003 Transforming graphite to diamond: An ab initio molecular dynamics study of graphite under shock compression

CHRISTOPHER J. MUNDY, Pacific Northwest National Laboratory, NIR GOLDMAN, I.F. WILLIAM KUO, EVAN J. REED, LAURENCE E. FRIED, Lawrence Livermore National Laboratory. ALESSANDRO CURIONI, IBM Research - Zurich. We present an extremely large scale ab initio calculation of the transformation of graphite to diamond under shock compression utilizing Car-Parrinello Molecular Dynamics (CPMD) in conjunction with the Multi-Scale Shock Method (MSSM). Our results indicate that the transition from graphite to diamond is Martensitic, in agreement with experimental observations. We find that a shock of 12 km/s forms a short-lived layered diamond phase which eventually relaxes to a cubic diamond structure. Moreover, access to the electronic structure allows the computation of electronic properties such as the x-ray absorption spectra (XAS) to characterize the final states. The XAS spectra and wide angle x-ray scattering spectra (WAXS) confirm the presence of a cubic diamond final state.

4:45PM J2.00004 Discussion Session: The Quality of Interaction Potentials in Molecular-Dynamics Calculations Under Extreme Conditions

B.L. HOLIAN, Los Alamos National Laboratory. How good are the interaction potentials used in classical molecular-dynamics (MD) simulations at high pressures and temperatures? A variety of semi-empirical functional forms have been used in large-scale MD simulations of shockwave phenomena, for example. These potential functions make possible more efficient large-scale simulations of extreme conditions than will (at least for some time to come) be possible by ab-initio quantum-mechanical (QM) MD. The potential-function parameters have traditionally been fitted to experimental properties at low pressures and temperatures, with little information contributed from experiments under extreme conditions. As a result, one can legitimately worry about the quality of MD simulations in such regimes. Modern computational capabilities have enabled the use of many more high-quality QM calculations for high-pressure, zero-temperature properties, which could be of considerable use in extending the phase space for fitting empirical parameters. However, one can ask whether these QM calculations are sufficiently accurate to aid the fitting process, and even more fundamentally, whether the current set of semi-empirical potentials even have the right functional forms. In addition, the effects of high temperatures on the fundamental physics (or chemistry) of the potentials used is almost entirely unexplored territory. Small-scale QM MD could contribute a great deal to this topic, if one were convinced of the quality of those simulations. It is hoped that the members of the audience who have had experience in using any of these semi-empirical potentials, or in generating QM data for fitting their parameters, will share some comments. The time is ripe for new paradigms in the exchange of information between QM and classical MD.

Tuesday, June 26, 2007 3:45PM - 5:30PM –
Session J3 Inelastic Deformation III
Fairmont Orchid Hotel Plaza I
simulations with this model reproduce well all details of observed behavior of the glass. Step-like compression demonstrate decreased impedance for further compression of cracked glass. The failure wave model includes equations of state of intact glass to longitudinal and bulk compression and release. The bulk compressibility of soda-lime glass was measured by the mixture method. It has been found that the ratio of average failure front velocity to rod penetration velocity decreases with increasing impact velocity (vp) in the range of vp = 0.4 to 2.8 km/s. As a consequence, the distance between the rod tip and the failure front is reduced with increasing vp. [1] Orphal DL, Behner Th, Hohler V, Anderson CE Jr, and Templeton DW, “Failure wave in DEDF and soda-lime glass during rod impact,” Shock Compression of Condensed Matter-2005, (M. D. Furnish, et al., Eds.), 1391-1394, AIP Conf. Series 845, Melville, NY, 2006.

The work was supported by the US Army Research Office, contract N62558-05-P-0113.
3:45PM J4.00001 Using the Heterodyne Method to Measure Velocities on Shock Physics Experiments1, OLIVER STRAND, Lawrence Livermore National Laboratory — Velocimetry is an important diagnostic for shock physics experiments. Velocities for these types of experiments can be in the kilometer-per-second range. We have developed a new velocimetry diagnostic for use on shock physics experiments that is based upon the heterodyne method. This diagnostic is easily assembled from commercially available parts developed for the telecommunication industry. The entire system uses simple mode fibers to transport the signals from the laser to the probes and back to the detectors. We mix the Doppler-shifted light from the moving surface with non-shifted light from the laser itself to generate a beat signal at the detector. For this system using 1550 nm lasers, a velocity of 1 km/s generates a beat signal of 1.29 GHz. The detectors and the digitizers must have high-bandwidth capabilities to faithfully follow the beat waveform to allow a determination of the frequency as a function of time. Our current system has a maximum velocity capability of over 5 km/s. This paper will describe the heterodyne velocimeter and will present some of the data that has been taken with it. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory, under contract No. W-7405-Eng-48.

1In collaboration with Tony Whitworth, Lawrence Livermore National Laboratory.

4:15PM J4.00002 Low-Power Heterodyne Velocimetry of shocked metal surfaces, ANDREW CRITCHLEY, ED PRICE, MARTIN PHILPOTT, NATHAN ROUTLEY, Hydrodynamics Division, DIAGNOSTICS DEVELOPMENT TEAM — A low-power variant of a Heterodyne Velocimeter (HetV) based on a LLNL design has been constructed to study motion of shocked metal systems. The system benefits from utilising a class 1 laser system enabling its safe usage and easy transfer between facilities. A number of experimental systems have been studied to establish the limits of the low power system including shocked metal targets on a large bore gas gun and H.E. driven systems. It is shown here how high quality absolute velocity measurements may be obtained from a variety of surface conditions without recourse to higher power lasers. Advanced analytical techniques have also been developed which complement the simple set-up and use of the HetV system which are presented here.

4:30PM J4.00003 Hugoniot and velocity history data using heterodyne techniques, P, ASOKA-KUMAR, R, CHAU, N.C. HOLMES, W.P. AMBROSE, K, KRAUTER, O.T. STRAND, J, NGUYEN, M, KUMAR, J, STOLKEN, LLNL — Heterodyne interferometry using Doppler-shifted coherent laser light offers a novel way to access the instantaneous velocity of a moving surface. Light scattered from a moving surface is shifted in frequency and when allowed to superpose with the original light will result in intensity modulation at the beat frequency of the two light fields. Such a system is capable of measuring shock arrival time and particle velocities in a gas gun experiment. We describe a 13-channel heterodyne interferometry system that measures shock arrival times in materials to a wide range of pressure values. The response time for shock arrival detection is similar to or better than the conventional pin recording system. EOS measurements from single crystal copper show no orientation dependence in the pressure range of 9-45 GPa. The U1-U2 relationship for all crystal orientations is consistent with previously reported data on polycrystalline copper. We compare velocity history data derived using several software analysis tools, short-time Fourier transform, Gabor transform, Wigner-Ville transform, and wavelet transform.

The work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

4:45PM J4.00004 Recent Advances in All Fiber Doppler Velocimeter at LSD. Xiang WANG, JIDONG WENG, HUA TAN, YUN MA, XIANMIN ZHOU, LABORATORY FOR SHOCK WAVE AND DETONATION PHYSICS RESEARCH TEAM1 — At LSD, we have developed series novel Interferometers and using these techniques to measure velocities up to several kilometers-per-second on different types of shock experiments for the past three years. These Interferometers possess of a very simple structure, which we called the All Fiber Velocimeter (AFV) and consist of some commercially available products developed for the telecommunications industry. We use a fiber laser and single mode fibers to deliver light to and from the target. The return Doppler-shifted light is mixed with the original laser light to generate a beat frequency proportional to the moving velocity. The beat signals were recorded directly onto fast digitized scope. Compared with traditional Optical Velocity Interferometer, such as VISAR or F-P, the AFV have more compact, reliable and less cost. This paper describes our applications to measuring velocities in shock or detonation experiments and presents recent data obtained with the AFV.

1LSD, Institute of Fluid Physics, CAEP, Mianyang 621900, Sichuan China

Tuesday, June 26, 2007 3:45PM - 5:00PM —
Session J5 Spectroscopy and Optical Studies II Fairmont Orchid Hotel Plaza III

3:45PM J5.00001 Raman Spectroscopy of RDX Single Crystals under Static Compression, ZBIGNIEW DREGER, YOGENDRA GUPTA, Washington State University — To gain insight into the high pressure response of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), an energetic crystal, Raman spectroscopy results were obtained for hydrostatic (up to 15 GPa) and non-hydrostatic (up to 22 GPa) compressions. These results are needed to properly interpret the shock data. Several distinct changes in the spectra were found at 4.0 GPa in the triazine region and at 10.3 GPa in the nitro region. The δ phase transition previously observed in polycrystalline samples. Symmetry correlation analyses indicate that the δ phase transition under shock wave loading has important implications for understanding the onset of chemical decomposition in shocked RDX. Work supported by DOE and ONR.

4:00PM J5.00002 Raman Spectroscopy Measurements in RDX Single Crystals Shock Compressed Along Different Orientations, JAMES PATTERSON, ZBIGNIEW DREGER, YOGENDRA GUPTA, Washington State University — Raman spectroscopy was used to examine the molecular level response of hexahydro-1,3,5-trinitro-α-triazine (RDX) single crystals to shock wave compression. Oriented single crystals were shocked under stepwise loading to peak stresses from 3.0 to 5.5 GPa. Changes in the Raman spectra of the CH stretching modes were monitored to determine the stress and orientation dependence of the shock response. Spectral shifts appeared to be similar for three crystal orientations below 3.5 GPa. Significant changes were observed in crystals shocked above 4.5 GPa. These changes were similar to those observed in static pressure measurements, indicating the occurrence of the α − γ phase transition in shocked RDX crystals. No measurable orientation dependence in the molecular response of RDX to shock compression was observed up to 5.5 GPa. The phase transition had an incubation time of about 100 ns when RDX was shocked to 5.5 GPa peak stress. The occurrence of the α − γ phase transition under shock wave loading has important implications for understanding the onset of chemical decomposition in shocked RDX. Work supported by DOE and ONR.
4:15PM J5.00003 Time-resolved products observed from high pressure deflagrating energetic materials using femtosecond IR spectroscopy. J.M. ZAUG, E.A. GLASCOE, J.C. CROWHURST, L.E. FRIED, M.R. ARMSTRONG, C.D. GRANT, Lawrence Livermore National Laboratory — What transient chemical species occur on the nanosecond to microsecond time-scale after an energetic material begins to deflagrate under Chapman-Jouguet conditions? What are the molecular lifetimes of transient species under similar conditions? Using ultrafast infrared spectroscopy to study the transient chemical phenomena of materials encapsulated in high-pressure diamond anvil cells (DACs), these and related questions can be addressed. Here we present a broadband time-resolved IR (TRIR) absorption technique applied to high-pressure deflagrating energetic materials. A 10 nanosecond laser pulse is introduced onto the surface of a high-pressure energetic material. After an induction period of approximately one microsecond the energetic material begins to deflagrate (1500–K) at subsonic velocities radially away from the laser ignited region. A mid-IR femtosecond laser pulse (pulse-gated, 2-10 micron tunable range) is transmitted through the deflagration front. The single-shot mid-IR absorbance is used to detect transient species. Our measurements provide a rigorous test of computational chemistry models.

4:30PM J5.00004 T-Jump/FTIR Studies of Poly-Glycidyl Nitrate (PGN) Pyrolysis. CHAD STOLTZ, SUHITHI PEIRIS, Naval Surface Warfare Center, Indian Head Division — The nitrate-ester binder PGN (poly-glycidyl nitrate) has a high oxygen balance and density, making it one of the most energetic nitrate ester binder systems for potential use. However, when cured using aliphatic isocyanate curing agents it ages poorly, hindering its applicability for use in energetic formulations. Scientists have end-modified the polymer chains with moieties that contain primary –OH groups in an attempt to increase post-curing stability. In an effort to understand the effects of hydroxyl end-modification and isocyanate curing, decomposition of PGN prepolymer has been investigated using T-Jump/FTIR (Fourier Transform Infrared Spectroscopy) of PGN allowing real-time analysis of decomposition gas products under simulated deflagration conditions. Our results identify decomposition products including: CH2O, H2O, CO2, CO, N2O, NO2, HCN and HONO. Kinetic rates relative to CO2 formation lead to calculated activation energies of 22 kcal/mol and 18 kcal/mol. Much higher activation energies (32 kcal/mol) were calculated relative to CH2O formation rates, in agreement with DSC data, indicating that CH2O formation is likely an initial decomposition step while CO2 formation is due to side gas phase reactions. Additional FTIR and optical microscopy studies indicate that condensed phase, backbone scission reactions also occur, causing time delays prior to major gas production.

4:45PM J5.00005 Ultrafast shock wave dynamics at high ambient pressure (∼10 GPa) in a diamond anvil cell 1. MICHAEL ARMSTRONG, JONATHAN CROWHURST, JOSEPH ZAUG, EVAN REED, WILLIAM HOWARD, Lawrence Livermore National Laboratory — The measurement and characterization of acoustic phenomena at high pressure is critical to the modelling of planetary dynamics, seismic events, and chemistry in extreme environments. Here we present the results of experiments using ultrafast laser excitation and detection of shock waves in metals in a diamond anvil cell (DAC) at ambient pressure up to at least10 GPa. Using ultrafast interferometry, we directly detect surface motion with less than 1 nm spatial resolution with 100 femtosecond time resolution. Notably, these experiments do not destroy the DAC, allowing multiple shot experiments at multiple pressures for a single DAC load. Such experiments enable examination of acoustic waves with significant strain (∼1%) starting at high ambient static pressure using a convenient, reusable and inexpensive apparatus.

1 This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

8:00PM - 8:00PM — Session K1 Poster Session II Fairmont Orchid Hotel Salon III

K1.00001 CONTINUUM AND MULTISCALE MODELING —

K1.00002 Critical Diameter Prediction for Steady Detonation in Gassless Metal-Sulfur Compositions. FRANCOIS-XAVIER JETTE, ANDREW HIGGINS, McGill University, SHOCK WAVE PHYSICS GROUP TEAM — Since many heterogeneous mixtures whose reaction products contain no gas are highly exothermic, a possibility exists for steady gassless detonation. Theoretical investigations have focused on approximating the product Hugoniot, which depends to a large extent on the amount of heat released and the volumetric expansion resulting from the reaction. If the products Hugoniot curve lies above the unshocked state on the pressure-volume plane, the Chapman-Jouguet tangency criterion gives the detonation velocity. Such Hugoniot analysis assumes that the rate of energy loss is negligible compared to the reaction rate, a condition approached only when the charge diameter is much greater than the critical detonation diameter. For charges of practical dimension, the lateral losses are not negligible. The current study accounts for the competition between lateral losses and reaction rate in order to predict the critical diameter of a mixture of manganese and sulfur. The reaction rate is based on experimental data obtained via temperature measurements during shock initiation of the mixture.

K1.00003 Composite Material Behaviour Under Shock Loading. R. VIGNIEVIC, J.C. CAMPBELL, P. HAZELL, N.K. BOURNE, Cranfield University, UK — Composite materials have been of significant interest due to widespread application of anisotropic materials in aerospace and civil engineering problems. For example, composite materials are one of the important types of materials in the construction of modern aircraft due to their mechanical properties. The strain rate dependent mechanical behaviour of composite materials is important for applications involving impact and dynamic loading. Therefore, we are interested in understanding the composite material mechanical properties and behaviour for loading rates between quasistatic and 1x108s⁻¹. This paper investigates modeling of shock wave propagation in orthotropic materials in general and a specific type of CFC composite material. The determination of the equation of state and its coupling with the rest of the constitutive model for these materials is presented and discussed along with validation from three dimensional impact tests.

K1.00004 DETONATIONS AND SHOCK INDUCED CHEMISTRY —

K1.00005 Thermodynamic and chemical behavior of benzene under shock conditions. JEAN-BERNARD MAILLET, NICOLAS PIÑEAU, EMERIC BOURRASSEAU, CEA-DAM — The thermodynamic and chemical behavior of benzene along its Hugoniot curve is investigated using Molecular Dynamics simulations with reactive potentials. The simulated Hugoniot curve is in good agreement with experimental data at low pressures. Moreover, the decomposition threshold is well reproduced. In the high pressure regime, reactive simulations show that benzene rapidly decomposes, but reacting pressures do not match experimental ones anymore. Simulations starting with diamond nanoparticles and hydrogen gas give good pressures along the Hugoniot. These simulations seem to confirm the existence of carbon clusters with diamond structure in the decomposition products of benzene.
K1.00006 Interaction between a steady detonation wave in nitromethane and geometrical complex confinement defects. , BLANDINE CROUZET, NOEL CARION, PHILIPPE MANCZUR, CEA-DAM Ile de France, BP12, 91680 Bruyères-le-Chatel — It is well known that detonation propagation is altered if the explosive is encased in an inert confining material. But in practice, explosives are rarely used without confinement and particular attention must be paid to the problem of explosive/confinement interactions. In this work, we have carried out two copper cylinder expansion tests on nitromethane. They differ from the classical cylinder test in that the liner includes evenly-spaced protruding circular defects. The aim is to study how a detonation front propagating in the liquid explosive interacts with the confining material defects. The subsequent motion of the metal, accelerated by the expanding detonation products, is measured using a range of diagnostic techniques: electrical probes, rapid framing camera, glass block associated with streak camera and velocity laser interferometers. The different experimental records have been examined in the light of a simple 2D theoretical shock polar analysis and 2D numerical simulations.

K1.00007 Shock Compaction of MnAs1-xSb x Powder using Underwater Shock Wave , YOUNG KOOK KIM1. Kumamoto University, HIROFUMI WADA, Kyushu University, SHIGERU ITOH, Shock Wave and Condensed Matter Research Center, Kumamoto University — MnAs1-xSb material is one of the ferromagnets which can contribute to a magnetic refrigeration system that is useable at room temperature. In order to obtain further high ferromagnetic properties with grain refinement, consolidation experiments of MnAs1-xSb powder is carried out by shock compaction using underwater shock wave. A water container which is a part of the shock compaction device is very important because the shock pressure distribution and the pressure magnitude of underwater shock wave depend on the shape of water container. Therefore, the water container is investigated numerically and experimentally in terms of the phenomenon of underwater shock wave. As result, we successfully obtained MnAs1-xSb bulk material by shock compaction using underwater shock wave, and the MnAs1-xSb bulk material is investigated in terms of magnetic properties.

1Corresponding Author

K1.00008 ABSTRACT WITHDRAWN

K1.00009 Research for Two-dimensional Critical Initiating State of Pressed TNT1, HUAN SHI, Guangzhou University, HUANG FENGLEI, Beijing Institute of Technology, TAN XIANQIAN, Guangzhou University — For two-dimensional(2-D) axial-symmetric non-steady detonation process, there is a considerable difference between an initiating and a failure process. The critical condition for both processes depends on the kind of explosive, the charge diameter, density and confinement, the initiating fashion, the inert additions and so on. In this paper, we have studied the 2-D critical initiating and failure conditions of pressed TNT charge. The critical initiating 2-D experiments have carried out for general granule, gross granule, casting and watered pressed TNT. The critical gap thickness has been used to compare with the relative shock initiating sensitivity. The pressure waves are got by manganese-constantan composite 2-D Lagrange sensor. The process of initiation and extinction has been calculated near the critical point by 2-D Lagrangian analysis method, and discussed the reason why exists the discrepancy. The results show that initiation and extinction are the entirely different dynamic process, which has little difference in original condition. It causes the pressure increase of the combustion peak’s rapid reaction behind precursor shock wave.

1Sponsored by the National Science Foundation of China -NSAF (10276015)

K1.00010 EXPERIMENTAL DEVELOPMENTS

K1.00011 Measurement of Shock Propagation and Metal Plasma Expansion in Underwater Wire Explosion by Utilizing CW Laser Light Source , SUNG-HYUN BAEK, EUN SOO LEE, INHO KIM, Agency for Defense Development, P.O. Box 35-5, Yuseong, Daejeon, 305-600, Korea — In order to get simultaneous high speed streak and framing images of exploding metal wires in water environment, we have employed cw green laser as a backlight source and laser beam splitter as a device separating images of exploding wires. By filtering the light emitted from the exploding wire with the help of a laser line filter, the images could become much finer than those taken with normal flash light source. The evolution and stability of the cylindrical plasma column together with the shock wave and metal plasma expansion speeds in water bath have been measured, and the data were applied to understand the plasma characteristics, e.g., electrical conductivity or thermodynamic properties of warm dense metal plasmas.

K1.00012 Decreasing Impact Tilt on a High Performance Two-Stage Gas Gun , M.E. BYERS, P.A. RIGG, J.S. ESPARZA, Los Alamos National Laboratory — There are four high-performance two-stage light gas guns in operation in the DOE complex. All four guns are similar in performance and diagnostics capabilities. Projectile velocity on these guns has typically been measured using a combination of magnetic coils and two frames of flash radiography. This requires that the projectile be in ‘free flight’ for a long distance (18 to 25 inches typical) in order to capture the projectile in flight. This leads to typical projectile tilt at impact in excess of 10 mrad. Recently, we have replaced the coil/x-ray system on the LANL high performance two-stage gun with Photonic Doppler Velocimetry (PDV) to obtain high accuracy (0.1%) projectile velocity measurements. This allows us to move the target very close to the end of the barrel to potentially decrease the impact tilt significantly. We will present the results of this study and compare them to the performance of the gun when the free flight section was present.

K1.00013 Detonation wave structure studies in high explosives by means of proton radiography , SERGEI KOLESNIKOV, SERGEI DUDIN, VICTOR MINTSEV, ALEXANDER UTKIN, Institute of Problems of Chemical Physics RAS, VICTOR DEMIDOV, ALEXANDER FERTMAN, ALEXANDER GOLUBEV, MARK KATZ, NIKOLAI MARKOV, BORIS SHARKOV, GENNADY SMIRNOV, VLADIMIR TURTIKOV, Institute for Theoretical and Experimental Physics — Proton radiography is the unique experimental technique for obtaining direct information about important material characteristics of real solid objects under dynamic conditions. The aim of the present work is the application of this method to the investigation of evolution of density in shock and detonation waves in high explosives (HE). Obtained information will be very useful for the improvement of existing detonation models and equations of state of HE. For this purpose a proton radiography facility for dynamic experiments on the basis of TWAC-ITEP accelerator is being constructed. A special containment chamber for explosive experiments was built. Static experiments with initiators of detonating HE charges were performed; as a result the proton radiographic images of initiators with time resolution of up to 10 ns were obtained. Dynamic experiments on the registration of detonation wave structure in pressed TNT are underway.

K1.00014 Confocal microscopy of water under static pressure , MATTHEW MCCLUKEY, BOBBIE RILEY, MICHAEL KNOBLAUCH, Washington State University — Developments in confocal microscopy have revolutionized the imaging of samples. Unlike conventional microscopes, which illuminate a wide area, confocal microscopes focus light onto a single spot on the sample. The sample is scanned by point, and an image is reconstructed from the data. Samples can be scanned in three dimensions, allowing one to obtain 3D image reconstructions. We have used confocal microscopy to obtain high-quality images of water freezing in a moissanite anvil cell. This technique could prove useful for a variety of equation-of-state investigations.
K1.00015 New Optical Diagnostics for Equation-of-State Experiments on the Janus Laser\textsuperscript{1}. DYLAN K. SPAULDING, UC Berkeley, DAMIEN C. HICKS, RAYMOND F. SMITH, JON H. EGGERT, Lawrence Livermore National Laboratory, R. STEWART MCMILLIAMS, UC Berkeley, GILBERT W. COLLINS, Lawrence Livermore National Laboratory, RAYMOND JEANLOZ, UC Berkeley — We report on the first implementation of both a streaked optical pyrometer (SOP) and nanosecond broadband reflectometry diagnostic for observation of ~1Mbar laser-driven dynamic compression experiments on the Janus laser at Lawrence Livermore National Laboratory. Temporally and spatially resolved optical pyrometry has been performed in the visible spectrum to measure self-emission from the sample in parallel with velocimetry and reflectivity measurements. A variety of materials have been investigated under ramp-compression (ICE) and shock-loading conditions with absolute temperatures obtained via a greybody comparison. Furthermore, a nanosecond, time-resolved, broadband reflectivity diagnostic has been successfully demonstrated and is being developed for permanent use in combination with pyrometry for equation-of-state measurements. Results from both diagnostics are discussed for materials including SiO2, diamond, MgSiO3 and MgO.

\textsuperscript{1}This work was performed under the auspices of the U.S. Department of Energy by UC Berkeley under Contract No. W-7405-ENG-48

K1.00016 Accurate measurement of shock front sharp in two-stage light-gas gun\textsuperscript{1}. XIANG WANG, CHENGDAI DAI, HUA TAN, QINGSONG WANG, JINGUI WANG, LABORATORY FOR SHOCK WAVE AND DETONATION PHYSICS RESEARCH TEAM\textsuperscript{2} — A two-stage light-gas gun is widely used for a variety of dynamic physics-property measurements up to 500 GPa or higher. The tilt and distortion of the impactor and of the resulting shock front have been precisely measured with sub-nanosecond resolution at the projectile velocities range from 2 to 7 km/s with Cu, Ta and Pt impactors. We report results of this proof-of-principle experiment and provide some comparison with simultaneously conducted point VISAR measurements.

\textsuperscript{1}This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W–7405–Eng–48.

K1.00018 Experimental and Theoretical Assessment of a Device Used for Evaluation of Blast and Fragmentation Effects, ANATOLY RESNYANSKY, SAMUEL WECKERT, Weapons Systems Division, Defence Science and Technology Organisation — An alternative to traditional momentum pendulum and pressure gages is sought to resolve an improved temporal response to blast and fragmentation and protect the evaluation device from damage when positioned closely to the source of blast. Evaluation concepts based on the use of strain gages have been used for some time in the scientific community. However, those devices either produce extensive parasitic oscillations or are restricted for use in close proximity to the source of the blast and during a short time only. An alternative design is suggested and analysed that can extend the analysis time to several milliseconds and can be used both in close proximity and at relatively large stand-off distances from the source of the blast. The device employs conventional strain gauges that are heavily protected from the blast and fragmentation. Numerical analysis demonstrates ways to minimise the system oscillations and these ways were partly implemented in the present system. A gas gun fitted with a diverging nozzle has been used to validate a version of the system, which was tested in the range of pressures representative of those occurring several meters from a moderate size explosive charge. The test results and simulation demonstrate the potential for using this type of devices in the field trial settings that involve the blast and fragmentation effects.

K1.00019 INELASTIC DEFORMATION, FRACTURE, AND SPALL —

K1.00020 Dynamic fracture and failure of silica glass: Void nucleation and growth, QI AN, School of Earth and Space Sciences, University of Science and Technology of China, SHENG-NIAN LUO, AARON KOSKELO, Los Alamos National Laboratory — We investigate dynamic fracture and failure of isotropic silica glass using classical molecular dynamics simulations, under both constant strain rate and shock wave loading. Two- and three-dimensional glasses were subjected to uniaxial and isotropic strains. We characterized the fracture and failure processes by following the nucleation and growth of nanovoids. The temporal and spatial evolutions of voids were quantified, and connected to classical nucleation and growth theories for fracture.

K1.00021 Front Face Spall of Concrete, ADAM COLLINS, DAVID CHAPMAN, WILLIAM PROUD, Cavendish Laboratory, University of Cambridge — Concrete cylinders (150 mm x 115 mm diameter) were impacted with half-inch steel spheres over a range of velocities (100 -500 m s\textsuperscript{-1}). Crater growth and debris cloud evolution were observed using high speed cameras aligned perpendicular and parallel to the impact direction. In-plane displacements of the impact face were tracked using Digital Speckle Photography (DSP). Radial cracking was seen to precede circumferential cracking on the high speed sequences and DSP showed bulk motion of fragments surrounding the impact zone. The profile images revealed no significant out-of-plane perturbations.

K1.00022 Study of Elastic Precursor Decay in ultra fine copper, STANISLAV FINYUSHIN, ANATOLY MIKHAILOV, ALEXEY FEDOROV, DMITRIY NAZAROV, TATIANA GOVORUNOVA, OLGA IGNATOVA — Laser interferometer was used to investigate elastic precursor decay in ultra fine copper M1 with the grain size of 110 microns. It is shown, that elastic precursor amplitude in ultra fine copper samples is in 2 - 3 times higher than in coarse-grained copper samples. The pressure of 12GPa. In this particular range of thickness elastic precursor amplitude decays from 1.87 GPa to 1.04 GPa. Ultra fine copper and coarse-grained copper M1 with the grain size of 110 microns were compared with respect to the elastic precursor decay values. It is shown, that elastic precursor decay in ultra fine copper is in 2 - 3 times higher than in coarse-grained copper samples.

K1.00023 Experimental Study on Shear Response of 92.93 wt% Alumina under Combined Pressure-Shear Loading, YAO GUOWEN, College of Civil Engineering and Architecture, Chongqing Jiaotong University, Chongqing, 400074, PR China, LIU ZHANFANG, Department of Engineering Mechanics, Chongqing University, Chongqing, 400044, PR China — Pressure-shear plate impact experiments and soft recovery experiments were performed for 92.93 wt% alumina with 75-mm-diameter compressed-gas gun. The in-material longitudinal and transverse particle velocities were traced by embedded electromagnetic velocity gauges. The decoupled transverse particle velocities show an attenuation of shear waves with decreasing of material shear rigidity. SEM analysis of intact samples shows heterogeneous meso-structures, and that of recovered samples shows the transit of intergranular microcracks to transgranular microcracks with increasing shock loading. Shear component promotes the microcracks nucleating and expanding, and these microcracks result in remarkable dilation of alumina samples after unloading.
K1.00024 Simulation of a Shock Recovery Experiment, K. HUGHES, Cranfield University, UK, R. VIGNJEVIC, N.K. BOURNE — It is difficult to obtaining experimental data for the behaviour of material under shock loading due to dynamic nature of this process and finite time available in which measurement can be taken. As a result shock recovery technique have been developed to allow examination of a material after shock propagation. The main goal of this experimental technique is to examine material properties after a single, well-defined shock wave followed by a single release wave have been introduced. The process should be such that any change found in the sample after recovery can only be attributed to the shock process alone. In order to achieve this, the geometry and design of the target and the fixture play an important role. In this work the simulations were performed using the Lagrangian hydrocode DYNA3D in order to size lateral and longitudinal momentum traps for the material being investigated. The investigation of the shock wave propagation in the simulation entails examining the stress, and velocity time histories for the whole fixture as well as for the single element, or block of elements of interest. In addition residual velocity of the sample was minimised to reduce its damage in the process of sample catching.

K1.00025 On Beryllium Deformation at High-Velocity Oblique Impact, ANATOLY MIKHAYLOV, RFNC-VNIIEF — At oblique impact of metals, intensive plastic shear strains and zones of strong heating are growing in neighborhood of contact point. Shear flows with velocity gradient depending on angle and velocity of impact of plates occur for short time. Due to intensive deformation, heating in local zones causes significant softening of substance. In these areas, shear modulus and yield strength are significantly less comparing to those at normal conditions. The mentioned effects result in distortion of profile of interface between metals after impact. Regular waves, non-symmetric distorted waves, melt layers of mixed components are formed. The process of high-velocity oblique impact of beryllium samples (beryllium and stainless steel) was experimentally studied. Though having low plasticity, beryllium has high ability for wave formation without significant plastic flow of material along sliding line (see fig.1). During high-velocity oblique impact of beryllium and stainless steel, their welded connection was achieved (see fig.2).

K1.00026 Feature in Accumulation of Microdefects in Copper Under Shock-Wave Loading, ALEXANDER PAVLENKO, ALEXANDER SHESTAKOV, ALEXANDER NURGALEV, DEMETRIUS KAZAKOV, RFNC-VNIITF — The microscopy and X-ray diffraction methods were used to investigate distribution of micro- and macro-defects in copper samples recovered after shock-wave loading. The electric gun GNBU was used to generate shock wave. Igniting effect of shock dynamics was recovered by the free surface velocity measured based on the Doppler shift in the wavelength of the probe laser radiation (IFP and push-pull VISAR technique). In-depth distribution of defects was compared for two modes of sample loading. In the first mode, samples were loaded by the shock wave whose amplitude was insufficient for spalling, which was initiated by the shock wave in the second mode.

K1.00027 Molecular dynamics study of tantalum spallation, LAURENT SOULARD, JOELLE BONTAZ, CEAM Ile-de-France, BP12, 91680 Bruyeres-le-Chatel — We present in this paper a molecular dynamics study of tantalum spallation. The spallation is the final stage of the damaging caused by a series of shock and rarefaction waves. This complex process is due to the nucleation, the growth and the coalescence of pores within a thin zone corresponding to the crossing of two rarefaction waves. Various experimental works allowed a partial description of this process. We present here a complementary analysis based on large classical molecular dynamics simulations in single and polycrystal of tantalum. We use a rather sophisticated potential function (MEAM) associated with multi-million particle samples. The simulations were made on the TERA 10 computer of CEA-DAM, and needed several hundred processors. We examine at various times the apparition and the evolution of pores, and provide their spatio-temporal distribution. The one dimensional (in the hydrodynamics sense) and 3D cases are considered in order to understand the effects of lateral rarefaction waves in the spallation phenomenon. Comparisons with experimental data are shown.

K1.00028 GEOPHYSICS AND PLANETARY SCIENCE

K1.00029 Measurement of the delayed failure in the shock compressed AOW rock, HONGLIANG HE, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, P.O.Box 919-102, Mianyang 621900, P. R. China, DENGPING CHEN, College of Science, Wuhan University of Technology, Wuhan 430070, P. R. China, FUQIAN JING, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, P.O.Box 919-102, Mianyang 621900, P. R. China — The failure property of AOW (Amphibolized Olivine Websterite) rock has been studied by measuring the velocity histories on the rear surface of the specimens at stresses much below the Hugoniot elastic limit. A delayed failure zone has been detected. It expands into the stressed material with a velocity comparable to the shock wave front, and follows the propagation of the shock wave with a time delay that decreases with the increasing of shock stress. The time delay is 1.2 microsecond at shock stress of about 0.9 GPa and 0.5 microsecond at about 3.7 GPa. A physical explanation considering the in situ activation and growth of the pre-existing microcracks by the local shear stress under shock wave is proposed. Comparisons with experimental data are shown.

K1.00030 Impact pressures generated by spherical particle hypervelocity impact on Yorkshire sandstone, KATARINA MILJKOVIC, EMMA TAYLOR, Open University, BILL PROUD, Cambridge University, KOSTAS TSEMBELIS, CHARLIE COCKE, JOHN ZARNECKI, Open University — We characterise the pressures achieved in spherical particle impact, as a precursor to investigating the possibility of shock-driven DNA modification in sandstone targets, which could occur at lower pressures than those previously established to cause extinction e.g. for B. subtillis [1, 2]. Hypervelocity impact experiments at 5 km/s using spherical chrome stainless steel projectiles onto Yorkshire sandstone were carried out using the Open University’s Hypervelocity Impact Facility [3]. Noting that the impact tests cannot be carried out in a completely sterile environment, we also establish the degree of background microbial contamination present by examining post-impacted targets. Hydrocode simulations (2-D and 3-D) are used to estimate the peak loading time and pressures as a function of target geometry, supported by 1-D hydrocode simulations using the CAV/KO software and published flyer plate data from the Cambridge Plate Impact Facility [4, 5]. [1] D. Stöffler et al, Icarus, 186 (2), 585-588, 2007; [2] M. J. Burchell et al, Mon. Not R. Astron. Soc., 352, 1273-1278, 2004; [3] E. A. Taylor et al, 37th ARA Conf, Sept 2006; [4] E. A. Taylor et al., APS 2005; [5] E. A. Taylor et al., ESTEC Impact Conf., May 2005.

K1.00031 ENERGETIC MATERIALS

K1.00032 FOX – 7 Cp PREDICTION FOX -7 Specific heat prediction from a proposed nominal / generic specific heat for CHNO energetic materials, JAMES BILLINGSLEY, U.S. Army RDECOM, Redstone Arsenal, AL 35898 — The importance of the specific heat (Cp) of CHNO energetic polymers relative to their impact shock sensitivity has been documented in U.S. Army technical reports and papers in the shock compression of condensed matter conferences. Another recent U.S. Army technical report (AMR-SS-06-35) documents a proposed nominal / generic (N/G) Cp for CHNO energetic materials. The motivation for this proposed N/G Cp was it’s utilization to predict Cp for energetic polymers whose Cp was unknown. The present paper documents the “successful” application of the (N/G) Cp concept to predict the Cp for a relatively new CHNO explosive, FOX-7. This application is called “successful” because it agrees very well with a more complex and sophisticated FOX-7 Cp prediction contained in the SCCM 2005 conference proceedings.
K1.00033 High-Rate Characterisation of Hexanitrostilbene — ROBERT CLARIDGE, QinetiQ Ltd, Fort Halstead, Sevenoaks, Kent, TN14 7BP, UK, ADAM PARKER, WILLIAM PROUD, University of Cambridge, Madingley Road, Cambridge, CB3 OHE, UK — Hexanitrostilbene (HNS) is a nitro-aromatic insensitive secondary explosive currently used in a number of insensitive munitions (IM) applications and under consideration for several others. The physical behavior of HNS is therefore important for the development of safe and reliable weapons systems. As a part of a comprehensive suite of shock characterisation experiments, one-dimensional plate impact experiments have been performed on HNS IV at two different densities. The unreacted Hugoniot curve was established at each density and the results compare to those reported in the literature. The data obtained from these experiments will assist in the modelling of ignition and growth within HNS based explosives systems.

K1.00034 Initiation of Polymer Bonded Explosive (PBXN-110) by Combined Shock and Shear Loading — JENNIFER JORDAN, Air Force Research Laboratory, Munitions Directorate, Eglin AFB, FL 32542, ROBERT DORGAN, Jacobs Technology, TEAS Group, Eglin AFB, FL 32542, MICHAEL NIXON, Air Force Research Laboratory, Munitions Directorate, Eglin AFB, FL 32542, RICHARD DICK, Shocks Unlimited, Albuquerque, NM — Combined shock and shear loading of explosives has been shown to result in detonation of explosives at input pressures less than those required with a nearly planar shock (Cart, APS-SCCM 2003). In this study, the effect of combined shock and shear loading on PBXN-110 is investigated. The explosive sample is loaded by a TNT/Octol plane wave lens in contact with a layer of PMMA followed by a cylindrical wave shaper that has one side angled at 45 degrees. The experiment is repeated for different thicknesses of the PMMA layer in order to vary the input pressure. In addition, the experiment is modeled using the Lagrangian finite element hydrocode EPIC, and the results of the experiments are compared with the numerical simulations.

K1.00035 The evolution of sensitivity in HMX-based explosives during the reversion from delta to beta-phase — PAUL PETERSON, KIEN-YIN LEE, DAVID MOORE, GABE AVLULCEA, LANL — In an effort to better understand the evolution of sensitivity in HMX-based explosives formulations during the reversion from delta to beta-phase, we have performed friction and impact experiments on a 3:1 mixture of Class 1 and Class 5 HMX. Initial baselines for Type 12 Drop Test. Impact and BAM friction sensitivities were taken for the beta-HMX. The HMX was then heated at approx. 180 degrees C for 14 hours. Raman spectroscopy was used to confirm the conversion to delta-phase. Impact and friction tests on the delta-HMX indicated a 20 percent increase in sensitivity for the delta-HMX in both impact and friction. Three weeks later we re-examined the HMX using Raman to determine the amount of reversion to beta-phase. However Raman spectroscopy indicated that the delta-HMX had instead converted to alpha-phase. Impact and friction test results were then repeated showing an additional 20 percent increase in sensitivity for the alpha-HMX. The alpha-HMX appears to be fairly stable over time as illustrated by Raman spectrum.

K1.00036 EQUATION OF STATE —

K1.00037 Shock Induced Equation of State of Polyvinylchloride — SIAN BUTLER, JEREMY MILLETT, AWE, Aldermaston, NEIL BOURNE, University of Manchester — The shock response of the common industrial polymer, polyvinylchloride (PVC) has been investigated by measurements of stress, shock velocity and particle velocity through embedded manganin stress gauges. Results in terms of shock and particle velocity show close agreement with published data within the literature. Stress measurements show an increasing difference with literature pressure values, but the calculated hydrodynamic pressure is in agreement with the literature. This suggests that the shear strength of PVC has a strong positive shock stress dependence.

K1.00038 The dissociation and thermodynamics of dense fluid oxygen by self-consistent fluid variational theory — Q.F. CHEN, Y. ZHANG, L.C. CAI, Y.J. GU — The dissociation, pressure, internal energy, and entropy of dense fluid oxygen at high temperatures and densities have been calculated from the free-energy functions using the self-consistent fluid variational theory. The accurate high-pressure and high-temperature effective pair potentials are adopted to describe the intermolecular interactions, which are made to consider molecular dissociation. In this paper, we focused on a mixture of oxygen atoms and molecules and investigated the phenomenon of pressure dissociation at finite temperature. The single-shock Hugoniot derived from this equation of state agrees well with gas-gun experiments for pressure vs. density. As density and pressure increase along the Hugoniot, the system undergoes a continuous transition from a molecular to a partially dissociated fluid containing a mixture of atoms and molecules. The equation of state and dissociation degree are predicted in the ranges of temperature of 5000- 16 000 K and density of 0.1-4.5 g/cm³. These data are formulated in the analytical form of dissociation degree-density-temperature and pressure-density-temperature equation of state.

1This work was supported by the National Natural Science Foundation of China (Grant No. 10674120).

K1.00039 Density Measurement Method of Isentropically Compressed Hydrogen at Megabar Pressures — NIKOLAY EGOROV, A. BYKOV, G. BORISKOV, YU. KUROPATKIN, N. LUKYANOV, V. MIRONENKO, V. PAVLOV, Russian Federal Nuclear Center - VNIEF — A radiography method of density measurement of condensed hydrogen at its isentropic compression up to megabar pressures is described in the paper. Experimental x-ray images of hydrogen compression devices in the megabar pressure ranges are presented. Measurement results of densities of condensed hydrogen and aluminum isotopes are presented. These results are used for hydrogen isotopes equations of state building.

This work was performed in the frameworks of the ISTC project # 2564.

K1.00040 The Effect of Fibre Orientation on the Shock Response of a Glass-Fibre Epoxy Composite — YANN MEZIERES, Assystem, JEREMY MILLETT, AWE, Aldermaston, NEIL BOURNE, University of Manchester — The response of a 2-D glass-fibre epoxy composite to one-dimensional shock loading has been investigated as a function of orientation of the fibres to the loading axis, in terms of the charge of state. When the shock axis is normal to the fibres, the response appears to be dominated by the epoxy matrix. In contrast, when the shock is parallel to one direction, the shock front appears ramped at low stresses, steepening as the impact stress increases. Analysis of these traces suggests that a low stress amplitude wave is transmitted along the fibres at a high velocity, with a lower velocity wave is transmitted through the matrix between those fibres, taking the material to its final stress amplitude.

K1.00041 The Hugoniot of Polychlorotrifluoroethylene — CHRIS STENNETT, Cranfield University, SUSAN SORBER, MALCOLM BURNS, JEREMY MILLETT, AWE, Aldermaston, NEIL BOURNE, University of Manchester — The shock response of polymers has attracted considerable interest of the past few years, in particular as they are often used as the binder phase in plastic-bonded explosives (PBXs). One such material, polychlorotrifluoroethylene (PCTFE) is used in just this application. It has also been used as an inert impedance match for some explosive compositions. Therefore there is a requirement that its response to shock loading be clearly understood. The work presented in this investigation examines the shock-induced equation of state in terms of stress, shock velocity and particle velocity. We also show that this material has an extremely high release speed, which must be accounted for when making comparisons with live compositions.

K1.00042 HIGH ENERGY DENSITY PHYSICS —
K1.00043 Self-similar flows in spherical geometry, JEAN GERIN-ROZE, CEA — If we are looking at the implosion of a sphere starting with a strong shock, the study of self-similar flows is a classical problem. We will assume that: - The sphere contains a perfect gas with a polytropic coefficient $\gamma = 5/3$. - The shock follows the equation: $r = A(t)^{-\gamma}$ with $t_0 < t < 0$. There are two known solutions to that problem: - The Guderley solution corresponding to $\alpha = \alpha_{ref} = 0.68838$. In this solution, the outer implosion velocity is almost constant and the compression rate at focalization is $p/p_0 = 0.6$. - The Y. Saillard solution corresponding to the same value of $\alpha$ (see SCCM-2005 Proceedings p515). In this solution, the outer velocity is increasing and the compression rate is tending to infinity. We will exhibit a new family of solutions: there is one solution for each value of $\alpha$ from 0 to $\alpha_{ref}$. As in the Y. Saillard solution, outer velocity and compressing rate are tending to infinity. These new solutions (with two parameters, initial outer velocity and shock shape coefficient $\alpha$) can provide us with benchmarks and perhaps also with ICF target design tool.

K1.00044 ISENTROPIC AND OFF HUGIONOT LOADING —

K1.00045 VELOCE - A Compact Pulser for Magnetically Driven Isentropic Compression Experiments, GILLES AVRILLAUD, MICHAEL DELCHAMBRE, JEAN GUERRE, FREDERIC BAYOL, FABRICE CUBAYNES, ITHPP, BORIS KOSVALCHUK, HCEI, MATHIAS BAYAV, JOE MERVINI, RICK SPIELMAN, ITI, JAMES ASAY, CLINT HALL, RANDY HICKMAN, TOMMY AO, SNL, MICHAEL WILLIS, KTECH, YOGENDRA GUPTA, JAMES ASAY, CORY BAKEMAN, WSU — Sharing similarities with the Gepli pulser dedicated to Isentropic Compression Experiments, Veloce, an even more compact electrical pulser has been designed and built in duplicate for SNL and WSU ($LxWxH=3.5x2.5x2m^3$). This type of machines complements gun facilities in the study of materials. In order to achieve a broad loading capability and fast turn around, the design is built around a solid dielectric transmission line to couple current from eight low inductance capacitors and switches. Peaking capacitors enhanced by a low inductance, multi-channel sharpening switch reduces the quarter period of the pulse down to 470 ns (0-100%). Gas mixtures in the switch cavity and inductances in parallel allow modifying the shape of the induced pressure wave. At 80kV of charge voltage, the peak current reaches approximately 3.5MA. Design of the pulser, range of pressures and velocities, as well as potential applications will be presented.

K1.00046 A numerical investigation of sleeved Taylor anvil specimens, J.C. CAMPBELL, Cranfield University, R. VIGNJEVIC, N.K. BOURNE — The Taylor anvil test is widely used for the validation of constitutive models in non-linear continuum mechanics codes. Numerical simulations have been performed on two modified specimen geometries: a sleeved cylindrical projectile and a sleeved conical projectile. In this study the core material is aluminium and the sleeve material is tungsten alloy, providing a large difference in impedance. The objective is to develop concepts that allow the stress profile along the axis of the projectile to be controlled and varied, allowing a greater range of material behaviour to be investigated through the core material is aluminium and the sleeve material is tungsten alloy, providing a large difference in impedance. The objective is to develop concepts that allow modifying the shape of the induced pressure wave. At 80kV of charge voltage, the peak current reaches approximately 3.5MA. Design of the pulser, range of pressures and velocities, as well as potential applications will be presented.

K1.00047 An investigation of surface velocimetry of shocked polyethylene using HetV, NATHAN ROUTLEY, ED PRICE, JEREMY MILLETT, AWE, Aldermaston, NEIL BOURNE, University of Manchester, ERIC BROWN, GEORGE GRAY, Los Alamos National Laboratory — The velocity history of a shocked free surface has traditionally been carried out using established techniques such as VISAR or Fabry-Perot. In recent years a third type of velocimetry has been developed by LLNL which uses Heterodyne techniques, PDV. This technique generates a Doppler beat frequency for low inductance reflected light incident on the surface and light internally reflected within the system. Unlike the other two techniques PDV does not use an interferometer, instead it relies upon having the ability to distinctly record the high beat frequency. The setting up and fielding of PDV is therefore much simpler. A low power (Class 1 laser) system using this principle, locally known as HetV, has been developed and assembled. A series of experiments has been carried out to investigate the Hugoniot of polyethylene using HetV and embedded stress gauges. The results obtained with HetV have been directly compared with the embedded gauge data from the same experiment.

K1.00048 Isentropic Compression Studies With High Explosive Pulsed Power, DOUGLAS TASKER, JAMES GOFORTH, HENN OONA, Los Alamos National Laboratory — An extensive study of the one-dimensional isentropic compression experiment (ICE), performed with High Explosive Pulsed Power (HEPP), has been completed at the Los Alamos National Laboratory (LANL); the findings will be summarized. The study has demonstrated that accurate, high pressure, isentropic Equations of State (EOS) data may be obtained with the HEPP-ICE technique. It will be shown that the HEPP-ICE target configuration is capable of producing magnetic pressures that are uniform to 1 part in 1000 over the central 87% of the sample faces, and that HEPP-ICE provides exact matching of the pressures between opposing samples; both of these features are key to obtaining accurate isentropic EOS data. An analysis of the overall accuracy of this technique will be given, together with the methods required for the highest accuracy. Isentropic EOS data have been obtained with the prototype LANL HEPP-ICE system, and the results for tungsten and copper will be presented. Moreover, some interesting structure was observed in the elastic to plastic failure of tungsten.

K1.00049 STRESS-STRAIN MEASUREMENTS —

K1.00050 The Response of Concrete to Shock-Loading, TONY ANDREWS, QinetiQ, UK, DAVID CHAPMAN, WILLIAM PROUD, University of Cambridge, UK — A series of plate impact experiments has been performed to assess the dynamic behaviour of dry and water saturated concrete. Information was obtained on the Hugoniot curve and dynamic shear properties using manganin gauges. This extends our previous data obtained on cement paste, mortar, and micro-concrete to full-size concrete. Despite the varying heterogeneous composition of concrete it has been found that all materials Hugoniot curves lie within a close range in pressure – particle-velocity space.

K1.00051 Incremental Stress-Strain Response of Polyomers Using Instrumented Reverse Taylor Impact Experiments, LOUIS FERRANTI, JR., NARESH THADHANI, Georgia Institute of Technology — Instrumented reverse Taylor impact experiments were conducted on pure epoxy and epoxy-cast Al$_2$Fe$_2$O$_3$ composites to determine the incremental stress-strain response under dynamic loading. High-speed camera images were used to measure transient (axial and areal) deformations and velocity interferometry was used to record complex elastic and plastic wave propagation behavior. For polymeric materials, elastic strains are generally not negligible compared to plastic strains and the rigid-plastic material behavior assumed in typical Taylor tests for metallic materials cannot be applied. Hence, in this work, a one-dimensional elastic-plastic wave propagation analysis developed by Hutchings to account for the appreciable elastic strains that can develop before the material yields, was used. The calculations obtain stress-strain behavior for each polymer composition and permit the characterization of internal elastic and plastic wave propagation response. These results are used to compare relative strengths between each composition and ascertain the influence particle reinforcement has on material properties.

$^1$ This work was supported by SNL and WSU.

K1.00052 Hugoniot of Geological Materials and relationships to static properties, A.R. GUEST, De Beers Group Services, C.H. BRAITHWAITE, W.G. PROUD, J.E. FIELD, Cavendish Laboratory, Cambridge University — The Hugoniot for a suite of rocks have been found through investigations carried out using a plate impact facility. These Hugoniots form the database for a numerical model used in the mining industry. It is of use to have a means of linking the quasi-static to the dynamic rock strength. Therefore, a series of comparisons have been made between the Hugoniot data and a variety of static tests. A characterisation method is suggested.

K1.00053 ABSTRACT WITHDRAWN

K1.00054 Deformation Twinning and Dynamic Strength of Copper During High-Rate Strain, VICTOR RAEVSKY, RFNC-VNIIEF — We will present the results of a study of the conditions under which microstructural changes involving the formation of complex bi-periodic twin structures occurs in copper during shock wave and high strain rate ($\dot{\varepsilon} > 10^7$ s$^{-1}$) shock-less loading. The overall morphology of the observed twin structures is rather complex, consisting of what we shall refer to as “packages,” with each “package” being composed of two sets of parallel twins aligned in a quasi-herringbone pattern. It is widely accepted that deformation twinning results in increased shear strength in samples recovered after shock wave loading. We have observed in this work a significant temporal component to the effect that these complex twin structures have upon shear strength. We have observed, for example, that the formation of these bi-periodic (herringbone-type) twin structures results in an initial loss of shear strength that is significant over a time period of about 0.2 to 0.4 $\mu$s. Following the initial loss of shear strength, deformation hardening produces an increase in shear strength that can be as great as several multiples of the initial value.

K1.00055 Strength of polyethylene, polypropylene and polystyrene behind a shock front, CHRISTINE TYLER, NEIL BOURNE, University of Manchester, JEREMY MILLETT, AWE, Aldermaston — There is a recent interest in the response of thermoplastics to shock. Previous work on three simple polymers has indicated that the shear strength increases as the complexity of the side group increases. Shear strength measurements have been conducted using lateral stress measurements with manganin gauges that have been recalibrated for use in the low stress regime. The present work aims to investigate the effect of configuration of the thermoplastic’s chain when side groups are added. In particular, whether steric effects are present when the groups become larger. Results show that whilst polyethylene has the lowest shear strength, polypropylene and polystyrene have similar values. In all cases the strength of polymer increases with time after the shock has past. As the applied stress increases, polystyrene and polypropylene strengthen to a higher degree when compared with polyethylene.

K1.00056 FIRST PRINCIPLES AND MOLECULAR DYNAMICS CALCULATIONS

K1.00057 Molecular dynamics simulation of shock-induced melting and alloying$^1$, SHIJIN ZHAO, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, TIMOTHY C. GERMANN, Applied Physics Division, Los Alamos National Laboratory, Los Alamos, NM 87545, ALEJANDRO STRACHAN, School of Materials Engineering, Purdue University, West Lafayette, IN 47907, LOS ALAMOS NATIONAL LABORATORY TEAM, PURDUE UNIVERSITY COLLABORATION — We observe sequent shock-induced melting processes occurring in Ni/Al nanonanimates by means of molecular dynamics simulations. We find a nice collaboration between the melting and alloying: the heat released from the exothermic alloying reactions facilitates the local melting in the respective Ni/Al bilayer, the liquid films from the local melting accelerate the exothermic alloying reactions. On the other hand, we uncover a keen competition between the melting and alloying from the overall pressure variation: the structural expansion upon melting leads to an increase of the pressure while the alloying reactions tend to decrease the pressure.

$^1$This work is supported by the Laboratory Directed Research and Development program (project no. LDRD-20050343ER) at Los Alamos National Laboratory, which is operated by Los Alamos National Security, LLC (LANS) under Contract DE-AC52-06NA25396 with US DOE.

K1.00058 MATERIALS SCIENCE

K1.00059 Updated Cask for Prevention against Possible Accidental Situations, ANDREY DRENNOV, RFNC-VNIIEF — Design of an updated cask for transportation of hazardous substances is suggested. This method allows us actually to exclude totally any risk at a fragment — bullet effect from outside. Namely, internal cavity of a standard cask with hazardous substance is filled with fine-dispersed loose material. An individual part of this material has high strength. At low velocities of a fragment (W $\leq$ 1.85 km/s), kinetic energy of this fragment is spared for heating and motion of microspheres. At average velocities (1.5 km/s $\leq W \leq$ 1.85 km/s), kinetic energy of a fragment is spared for heating, motion, and work for collapse of some microspheres. At high velocities (W $>$ 2 km/s), the effect of super deep penetration occurs. If to connect the coordinate system with a moving fragment, we will get a steel target and several echelons of microparticles moving towards this target with high velocity. Since there are a lot of particles, the effect of super deep penetration occurs many times. Fragment is consecutively fragmented to sizes corresponding to sizes of microspheres.

K1.00060 Hugoniot Measurement on a Gel-binder system, RAY FLAXMAN, WILLIAM PROUD, Cavendish Laboratory, University of Cambridge, CAROLINE HANDLEY, AWE, Aldermaston, UK, DAVID CHAPMAN, Cavendish Laboratory, University of Cambridge — Gel systems are finding increasing use in composites where a degree of compliance with limited residual stress is required. In this poster the results of a series of plate impact experiments are presented. The material has been characterised to obtain the principal Hugoniot, this is compared to the points obtained from a ring-up experiment, the effects of the shock heating are seen.

K1.00061 Dynamic compaction of iron disilicide powders, VLAYER LASHKOV, RFNC - VNIIEF, Sarov, Russia, ALEXANDER SELEZENEV, ANDREY STRIKANOV, ANYA TIKHONOVA, VLADIMIR RYBAKOV — Iron disilicide is attractive material for semiconductor thermoelectric cells. When made mechanochemically, the ground disilicide is very difficult to compact, which is particularly the case for nanopowders. This is a technology problem that seriously hinders the use of this material in industry. The work presented in the paper is where dynamic compaction method is used for compacting iron disilicide powder. Specific feature of this method is that the powder to be compacted is placed into a metal container, which is exposed to shock wave pressure from detonating HE. Dynamic compaction of the powder can produce strong chemical bonds at the contact between material grains, which is an advantage of this method. An experimental dynamic compaction setup has been developed that provides variation of the shock wave pressure from a few to dozens of GPa. The experiments were performed there using plane shock loading of a pre-compactod cylindrical iron disilicide sample in metal container surrounded by a thick frame of steel. The experimental dynamic compaction setup has been developed that provides variation of the shock wave pressure from a few to dozens of GPa. The experiments were performed there using plane shock loading of a pre-compactod cylindrical iron disilicide sample in metal container surrounded by a thick frame of steel. The experimental dynamic compaction setup has been developed that provides variation of the shock wave pressure from a few to dozens of GPa. The experiments were performed there using plane shock loading of a pre-compactod cylindrical iron disilicide sample in metal container surrounded by a thick frame of steel. The experimental dynamic compaction setup has been developed that provides variation of the shock wave pressure from a few to dozens of GPa. The experiments were performed there using plane shock loading of a pre-compactod cylindrical iron disilicide sample in metal container surrounded by a thick frame of steel.
K1.00062 High Pressure Equation of State of a Zirconium-Based Bulk Metallic Glass\textsuperscript{1}, MORGANA MARTIN, Georgia Tech, TOSHIKORI SEKINE, TAKAMICHI KOBAYASHI, National Institute for Materials Science, LASZLO KECSKES, Army Research Laboratory, NAOHARU THADHANI, Georgia Institute of Technology — The high pressure $U_s - U_h$ Hugoniot equation of state of ($Zr_{27}$Nb$_{2}Cu_{15.4}$Ni$_{12.6}$Al$_{10}$ bulk metallic glass (BMG)) was determined using plate impact experiments. The National Institute for Materials Science (NIMS) two-stage light-gas gun was utilized for the high pressure measurements (~26-115 GPa) and the Georgia Institute of Technology (GT) single-stage gas gun was utilized for the relatively low pressure measurements (~5-23 GPa). NIMS experiments were instrumented with streak photography and the inclined mirror method to simultaneously measure shock velocity and free surface velocity. GT experiments utilized polynitride fluoride (PVDF) stress gauges and velocity interferometry (VISAR) to simultaneously measure the shock velocity, free surface velocity and stress. Results from the streak camera records and PVDF gauges + VISAR traces, as well as impedance matching calculations, were used to generate the $U_s - U_h$ Hugoniot equation of state data and determine the high pressure stability of the BMG. \textsuperscript{1}ARO Grant No. E-48148-MS-000-05123-1 (Dr. Mullins program monitor), NSF EAPSI Program, NASA Jenkins Fellowship

K1.00063 Microstructures produced by dynamic friction\textsuperscript{1}, CHRIS POULTER, RON WINTER, AWE, Aldermaston, Reading, UK, HONG JIN KIM, Materials Science and Engineering, OSU, Columbus, OH — An experimental technique in which an explosive charge induces sliding between two metals has been developed as part of a study of dry friction at very high sliding velocities and pressures. Aluminium alloy/stainless steel and pure aluminium/pure copper tribo-pairs have been investigated. Optical studies of cross-sections of the aluminium samples have shown that, depending on the stress/slip velocity conditions, the sub-surface deformation is either deep, suggesting high friction, or concentrated near the surface suggesting low friction. Recent further studies of the microstructure near the surface of the samples are described. Transmission electron microscopy reveals that a clearly delineated layer of nanocrystalline material about 1 micron thick is developed at the surface of the aluminium samples. Spectroscopic analysis shows evidence of inter-penetration of the two materials with mixing occurring at a very fine scale. The observations support the contention that, in a mechanism akin to adiabatic shear, thermal softening of the material at the sliding interface plays a key role in shock-induced friction. \textsuperscript{1}Professor emeritus of Kobe University of Mercantile Marine

K1.00064 Semi-Empirical Model for the Electrical Behavior of Explosively Driven Ferroelectric Generator , MINSU SEO, MYUNG-HWAN PARK, INHO KIM, Agency for Defence Development, P.O. Box 35-5, Yuseong, Daejeon, 305-600, Korea — Ferroelectric ceramic compressed by a strong shock releases a large amount of bound surface charges and it is the reason why it has been widely utilized in compact pulse power devices. The origin of charge release from the ceramic has not known clearly but inferred as either domain reorientation or stress induced phase transition. In this work we introduce a semi-empirical model to describe the electrical behavior of explosively driven ferroelectric generator. A PZT ceramic is considered as a ferroelectric material into which the shock wave is induced normally to its polarization vector. A series of experiments has been performed to obtain the shocked properties of PZT. The parameters in the semi-empirical model have been determined from measurement. A comparison of the calculated and experimental results for both resistive and capacitive loads shows in good agreement.

K1.00065 Discharge of PZT 95/5 Ferroelectric Ceramics under Tilted Shock Wave Compression\textsuperscript{1}, FUPING ZHANG, JINMEI DU, YI ZHANG, YUSHENG LIU, GAOMIN LIU, HONGLIANG HE — The current waveform of Ferroelectric ceramics PZT 95/5 depoling under tilted shock wave compression has been studied. Analytic model was established to analyze the effects of incident angle on the rising time, duration and peak amplitude of the depoling current. Experiments were conducted as well to confirm these effects. Result indicted that with the increasing of incident angle, the depoling current rises with longer time, pulse duration becomes broad and the peak amplitude keeps constant until the waveform decays into triangular form. \textsuperscript{1}Professor emeritus of Kobe University of Mercantile Marine

K1.00066 OTHER TOPICS —

K1.00067 Jumps across an outgoing spherical shock wave front\textsuperscript{1}, YUKIO SANO\textsuperscript{2}, TOMOKAZU SANO, Osaka University — Two types of jump equations are derived from the equations of conservation of mass and momentum in a moving coordinate system and in the inertial coordinate system. The first equations, of Rankine-Hugoniot (RH) type, show that the geometrical effect may be neglected at distances of movement of the rear of the wave front that are more than ten times as long as the effective wave front thickness. Furthermore, using conditions required to satisfy the RH jump conditions, which are shown by the RH type equations, a method is developed to judge the applicability of the RH jump conditions to the jumps. The second equations are those of general form obtained by expressing a volumetric strain wave $\varepsilon$ in the wave front by any form. In the neighborhood of the center of the wave front, for $\varepsilon < -0.09$, radial particle velocity in the jump in any materials is inversely proportional to the square of a dimensionless distance from the center to the rear, and for $\varepsilon < -0.04$, radial stress in the jump in some viscous fluids and solids is inversely proportional to the distance. In conclusion, an outgoing spherical wave front attenuates greatly near the center due to the geometrical effect as well as rarefaction waves overtaking from behind, while the geometrical effect is negligible at the specified positions that are distant from the center. \textsuperscript{2}Professor emeritus of Kobe University of Mercantile Marine

K1.00068 Reevaluation of the precursor decay anomaly in single crystal lithium fluoride\textsuperscript{1}, YUKIO SANO\textsuperscript{1}, TOMOKAZU SANO, Osaka University — The precursor decay anomaly in single-crystal lithium fluoride has been reevaluated by estimating dislocation densities along the Sano’s decay curve $[\text{San}\!, \text{ J. Appl. Phys. 85, 7616 (1999)}]$ that are much lower and slower than the Asay’s decay curve $[\text{Asay et al., J. Appl. Phys. 43, 2132 (1972)}]$. It is demonstrated that the density at the leading edge of the follower depends only on the slopes of the decay curves for particle velocity and stress, irrespective of the form of the follower and the slope at the leading edge. The maximum dislocation density at the beginning of the decay process is about 1/22 times as large as that estimated along the Asay’s decay curve. Thus, the anomaly is reduced significantly. In addition, by estimating the density at the rear of the precursor, it is also shown that a large number of dislocations are multiplied in the vicinity of the leading edge of the follower. This increase in dislocation may be responsible for the multiplication of dislocations at the subgrain boundaries in the bulk as well as that of initial dislocations in the bulk. \textsuperscript{1}Professor emeritus of Kobe University of Mercantile Marine

K1.00069 Dynamic yielding behind near-steady precursors\textsuperscript{1}, YUKIO SANO\textsuperscript{1}, TOMOKAZU SANO, Osaka University — In materials where shocks induce large shear stresses, plastic flow occurs and the stress state becomes more isotropic. The resulting compressibility change causes a single shock wave to be unstable and to separate into a precursor and a follower, which is followed by a plastic wave. The analysis performed here demonstrates that followers I, II, R', and Rb appear in the decay process of the precursor in sequence, and that dynamic yielding occurs at the leading edges of the followers I, II, R', and Rb. Here the followers C, I, II, R', and Rb are the contraction wave, the degenerate contraction waves I, II, the sub-rarefaction wave R', and the rarefaction wave Rb. \textsuperscript{1}Professor emeritus of Kobe University of Mercantile Marine

K1.00070 PHASE TRANSITIONS —
K1.00071 A Multi-Phase Equation of State for Bismuth. GEOFFREY COX, AWE — This paper considers a multi-phase equation of state for bismuth. At a phase transition there are changes in volume, energy, and properties of a material that should be included in an accurate model. Modifications are made to a previously published EoS [1] with the aim of extending the pressure and temperature range of the EoS and producing a reasonable estimate of shock melt. This new EoS contains five solid phases and a liquid phase. Comparisons are shown between experimental data and the modified and unmodified EoS.


K1.00072 Shock-Melting of Tin from Sound Velocities Measurements. JIAN BO HU, XIAN MING ZHOU, HUA TAN, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang 621900, SHOCK WAVE PHYSICS TEAM — In this paper, an improved reverse-impact technique was used to measure sound velocities of tin at the pressure range of 37GPa ~ 80GPa, using time-resolved velocity interferometer system for any reflector (VISAR). Bulk and longitudinal sound velocities can be obtained simultaneously by this technique with the precision of about 5% and 2%, respectively. Experimental results are consistent with the thermodynamic calculations for the γ phase of tin. Results also show elastic-plastic transition in the release process disappears gradually and longitudinal sound velocity is changed gradually to bulk sound velocity with Hugoniot stress increasing. In combination with phase diagram of tin, it is suggested that pre-melting is occurred before the bulk melt because of the energy deposition at the grain boundary. Only the location of completely shock-melted state can be determined from sound velocities measurements.

K1.00073 Retention of the Alpha-Prime Phase in a Pu-Ga Alloy After Hydrostatic Compression. A.J. SCHWARTZ, M.A. WALL, D.L. FARBER, K.T. MOORE, K.J.M. BLOBAUM, Lawrence Livermore National Laboratory — Delta-phase Pu-Ga specimens, 2.3 mm diameter by 100 microns thick were compressed to approximately 1 GPa in a large volume moissanite anvil cell to induce the transformation to the alpha-prime phase. The recovered samples were characterized at ambient pressure with optical microscopy, x-ray diffraction, and transmission electron microscopy. Optical microscopy revealed a very fine microstructure that appears to be single phase. The preliminary conclusion was supported by x-ray diffraction, which showed only the monoclinic reflections from the alpha-prime phase. However, transmission electron microscopy revealed small regions of delta-phase with a very high dislocation density. From these results, we conclude that hydrostatic compression to 1 GPa is not fully sufficient to fully support by x-ray diffraction, which showed only the monoclinic reflections from the alpha-prime phase. However, transmission electron microscopy revealed small regions of delta-phase with a very high dislocation density. From these results, we conclude that hydrostatic compression to 1 GPa is not fully sufficient to form and retain 100% alpha-prime.

K1.00074 Surface Specularity as an Indicator of Shock-Induced Solid-Liquid Phase Transitions. G.D. STEVENS, S.S. LUTZ, W.D. TURLEY, L.R. VEESER, NSTec Special Technologies Laboratory, P.A. RIGG, B.J. JENSEN, R.S. HIXSON, Los Alamos National Laboratory — When high density solid metals melt upon release after shock loading, they exhibit a number of features that suggest that significant surface changes accompany the phase transition. The reflection of light from such surfaces changes from specular (pre-shock) to diffuse upon melting. A familiar manifestation of this phenomenon is the loss of signal light in velocimetric measurements typically observed above pressures high enough to melt the free-surface. Unlike many other potential material phase-sensitive diagnostics (e.g., reflectometry, conductivity), changes in the specularity of reflection provide a dramatic, sensitive indicator of the solid-liquid phase transition. Data will be presented from multiple diagnostics that support the hypothesis that specularity changes indicate melt. These diagnostics include shadowgraphy, infrared imagery, high-magnification surface images, interferometric velocimetry, and most recently scattering angle measurements.

K1.00075 Phase Transformations of Graphite at Shock-Wave Loading in Steel Targets with Conic Cavities. ANDREY ZHUK, JIHT RAS, ALEXANDER CHARAKCHCHYAN, Dorodnicyn Computing Center RAS, VLADIMIR MAILYAVSKYI, KONSTANTIN KHISHCHENKO, DMITRIY ZHERNOKLETOV, TATIANA BORODINA, GEORGIY VALIANO, IHED of JIHT RAS — Phase transformations of graphite with various densities and microstructure at shock-wave loading in steel targets with conic cavities were studied. Graphite GMZ (ρ=1.70 g/cc), MPG-7 (ρ=1.91 g/cc) and MF-307 (ρ=2.01 g/cc) were used in the experiments. The recovered specimens were studied by means X-ray phase analysis. The maximal degree of graphite-diamond transformation having a place in the experiments was estimated. The detailed data was compared to results of 2D numerical modeling. The detailed description of the numerical methods is presented in [1]. We have found that with growth of a degree of three-dimensional regularity and a size of crystal grains of graphite, transition onset pressure and speed of phase transformation falls. [1] V.V. Milyavsky, V.E. Fortov, A.A. Frolova, K.V. Khishchenko, A.A. Charakhchyan, L.V. Shurshalov, Comp. Math. & Math. Phys. 46 (2006) 873.

K1.00076 SPECTROSCOPY AND OPTICAL STUDIES –

K1.00077 Optical Shock Generation Integrated with Time-resolved Spectroscopy. G. SAINI, T. PEZERIL, MIT, ISN, S.E. KOOI, ISN, E.L. THOMAS, K.A. NELSON, MIT, ISN — A detailed understanding of how materials respond to ballistic shock-loading is critical for the design and development of new protective materials. However, nonlinear viscoelastic deformation present in polycrystals during and immediately following a ballistic impact event is not currently well understood. The dynamic mechanical responses of materials during shock-loading are quite complex, with large amplitude compressions resulting in strain rates of 10^9 s^-1 and pressures exceeding several GPa. The mechanical properties of multilayered thin films are measured using impulsive stimulated thermal scattering, a laser-based photoacoustic technique. Since the data can be acquired on a single shot basis, the measurement is compatible with laser shock loading. To this end, a novel pairing of optical shock generation and time-resolved spectroscopy is used, providing an insightful tool for studying the material response to large-amplitude short-time mechanical transients. Laser-induced shock loading has been synchronized with ISTS measurement of acoustic waves so that dynamical evolution of mechanical properties in laser-shocked materials can be examined. The results could complement those from a recent gas gun-ISTS combination that permits measurement of acoustic and mechanical properties during steady-state shock loading. This work is supported by the U.S. Army Research Office.

K1.00078 Simulating EXAFS Patterns of Shocked Crystals. ANDREW HIGGINbothAM, University of Oxford, UK, ROBERT ALBERS, TIM GERMANN, BRAD HOLIAN, KAI KADAU, PETER LOMDAHL, LANN, WILLIAM MURPHY, JUSTIN WARK, University of Oxford, UK — Extended X-ray absorption fine structure (EXAFS) can be a useful tool in structural determination for solid state systems. Simulation of signals from EXAFS experiments using FEFF is usually carried out using the FEFF package. Although fast, the standard FEFF approach is based on perfect crystals and includes temperature effects using a Debye model. In the case of a shocked crystal it is not clear that such a simulation can encapsulate the full physics of the system, especially if mixed crystallographic phases, dislocations or grain boundaries have a significant effect on the signal. Molecular dynamics (MD) can provide detailed information on these features in many shocked materials of interest and so an EXAFS averaging technique based on MD data could allow a more meaningful comparison with experimental data. We will present a comparison of the standard FEFF approach with a configurational averaging technique based on MD data. The relative merits of the two methods will be highlighted and the implications for simulating EXAFS spectra for shocked samples discussed.
K1.00079 Prospects for Using X-Ray Free-Electron-Lasers to Investigate Shock-Compressed Matter1, BOB NAGLER, ANDREW HIGGINbotham, GILES KIMMINAU, WILLIAM MURPHY, JUSTIN WARK, THOMAS WHITCHELER, University of Oxford, UK; JAMES HAWRELIAK, DAN KALANTAR, RICHARD LEE, HECTOR LORENZANA, BRUCE REMINGTON, LLNL; JORGEN LARSSON, University of Lund, Sweden, NIGEL PARK, AWE, Aldermaston, UK, KLAUS SOKOLOWSKI-TINTEN, University of Duisburg-Essen, Germany — Within the next few years hard X-ray Free Electron Lasers will come on line. Such systems will have spectral brightnesses ten orders of magnitude greater than any extant synchrotron, with pulse lengths as short as a few femtoseconds. It is anticipated that alongside the X-ray source large-scale optical lasers will be sited, capable of shock-compressing matter to multi-megabar pressures. We discuss the opportunities that such systems may afford to further our knowledge of shocked and isochorically heated matter, in particular investigating the potential to perform small angle and/or diffuse scattering that may allow in situ measurements of dislocation densities in shocked crystals, and the creation of warm dense matter.

1 BN is supported by the EU Marie-Curie RTN ‘FLASH’

Wednesday, June 27, 2007 8:00AM - 10:00AM
Session L2 Material Science II Fairmont Orchid Hotel Amphitheater

8:00AM L2.00001 Dislocation Mechanics Under Extreme Pressures, RONALD ARMSTRONG, University of Maryland, WERNER ARNOLD, TDW-MBDA Systems, Germany, FRANK ZERILLI, NSWC IHD, Maryland — The shock-induced plasticity of copper, Armco iron, and tantalum materials is attributed to strain rate control by a substantial dislocation density being generated at the shock front. A thermal activation type constitutive equation is employed for the dislocation generation based on achievement of a limiting small activation volume for the process. A linear dependence of the equivalent compressive stress on logarithm of the plastic strain rate is predicted. The prediction compares favorably with Swegle-Grady and Meyers measurements previously fitted to a power law relationship. For Armco iron and tantalum, control is matched with a dislocation description of deformation twinning at the shock front. By comparison, the uniform shock-less loading in an isentropic compression experiment (ICE) provides for plastic strain rate control by the drag-resisted movement of mobile dislocations within the resident dislocation density.

8:15AM L2.00002 Initial Temperature Effects on the Shock Compression and Release Properties of Different Alumina-Filled Epoxy Compositions1, MARK ANDERSON, DAVID COX, STEPHEN MONTGOMERY, ROBERT SETCHELL, Sandia National Laboratories — Alumina-filled epoxies are composites having constituents with highly dissimilar mechanical properties, resulting in complex behavior during shock compression and release. Two distinguishing characteristics are amplitude-dependent wave structures and high release velocities. Recent studies examined the effects of various compositional changes on these shock properties. As expected, the strongest effects were observed when the total alumina volume fraction was reduced in steps from a nominal 43% to 0%. In the present study, compositions prepared over the same range of alumina loadings were examined at initial temperatures from -50 to 70 °C. Laser interferometry and wave timing were used to obtain transmitted wave profiles, Hugoniot states, and release wave velocities. Initial densities were determined from thermal expansion coefficients measured for each composition. Although initial density changes are very small, significant temperature effects on wave speeds and Hugoniot states were observed.

1 Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration.

8:30AM L2.00003 Taylor Impact Of Ti-6Al-4V, SAM MCDONALD, NEIL BOURNE, University of Manchester, GEORGE GRAY, Los Alamos National Laboratory; JEREMY MILLETT, GLENN WHITEMAN, AWE, Aldermaston — Over the past few years, a body of work has been performed to investigate the response of the titanium-based alloy, Ti-6Al-4V to one-dimensional shock loading. In this report, we take this work further including measurements of the shock response of the materials to one dimensional loading and by examining the behaviour of right cylinders of this alloy to high velocity impact onto a rigid surface with multi axial loading. The results have been analyzed using a variety of techniques. In particular this work focuses on X-ray tomography that has been used to examine void formation immediately below the impact face due to interactions of releases, and other microstructural features from the cylinder edges.

8:45AM L2.00004 Using Laser Induced Shock Waves to Investigate The Nanoparticle Transition From Bulk Behavior to Discrete Atom/Finite Size Behavior1, BERNARD GERSTMAN, Florida International University — As particle size becomes smaller, finite size effects become important and thermo-mechanical properties of nanoparticles, such as the bulk modulus, deviate from the values of larger size particles. The change in properties for the bulk modulus is important from an applied standpoint as nanoparticles are used in various applications and also important for testing fundamental models of atomic interactions in finite size systems. We develop a first principles model to predict all thermo-mechanical effects generated by any laser pulse incident on a nanoparticle. The use of short enough pulses produces shock fronts in the surrounding transparent medium that the nanoparticles are immersed in, such as water or a solid polymer. We show that, using particles of decreasing size, measurements of these shock fronts in the medium allow the determination of the size at which a nanoparticle is small enough to deviate from its bulk behavior and manifest finite size effects. Because the measurements can be made in the surrounding medium, they are easier to perform experimentally.

1 The author thanks the AFOSR for Grant F49620-03-1-0221.

9:00AM L2.00005 Influence of Peak Shock Stress on the Quasi-static Reload Response of HCP Metals, E.K. CERRETA, Los Alamos National Laboratory, G.T. GRAY III, C.P. TRUJILLO, D.W. BROWN, C.N. TOME — Textured, crystal-bar-purity hafnium has been shock loaded at 5 and 10 GPa, below the pressure reported for the α → ω phase transformation, 23 GPa. The specimens were “soft caught” for post-shock characterization. The substructure of the shocked materials was investigated through optical and transmission electron microscopy and the texture evolution was probed with neutron diffraction. Shocked materials were reloaded quasi-statically in compression. The deformation behavior of as-pressed hafnium under quasi-static conditions is compared to its response following shock prestraining. The reload response is correlated to differences in defect density due to shock loading and compared with similar observations in other HCP metals. The microstructural development during quasi-static loading of the preshocked specimens is compared to that of the as-annealed specimens.

9:15AM L2.00006 A Study of phase explosion of metal using high power Nd:YAG laser ablation, JACK Y. YOH, HYUNHEE LEE, KIHONG KIM, Seoul National University — The high speed blast wave generated by the laser ablation of metal reaches a propagation velocity of several thousand meters per second. The strikingly similar flow conditions to those of detonation wave allow one to apply the governing equations of motion for energetic materials to understand the explosive behavior of metal surface upon laser ablation. We describe the high power (>2.5 J/pulse) laser ablation technique for generating phase explosion for selective metals. The time resolved shadowgraph images of explosive wave fronts show that the point source (the targeted beam spot) blast wave radius is consistent with that given by the classical Sedov-Taylor solution. A multi-material shock physics code originally developed for high explosive detonation is applied for the full simulation of metal ablation based phase explosion. Some details on the experimental setup and the work-in-progress calculations are given.
9:30AM L2.00007 Dynamics of the Onset of Damage in Metals under Shock Loading\(^1\), AARON KOSKELO, SCOTT GREENFIELD, KENNETH MCLELLAN, DARRIN BYLER, ROBERT DICKERSON, DENNIS PAISLEY, SHENGNIU LUO, DAMIAN SWIFT, DAVIS TONKS, Los Alamos National Laboratory, PEDRO PERALTA, Arizona State University — We seek to understand the development of damage in polycrystalline materials under shock loading. Our current focus is on the role material microstructure plays in spall formation. Our approach is to use sensitive dynamic interferometry methods (see Greenfield’s and Paisley’s presentations at this meeting) to probe surface displacement and velocity dynamics of copper during shock loading using laser-launched flyers. Specimens have either columnar grains or have no more than one or two grain-boundaries between the spall layer and the surface that is monitored. In this way, we expect to unravel the complex surface dynamics observed in terms of loci for damage within the material. The dynamic measurements are to be correlated with pre- and post-shot materials characterization and damage assessment. Variables such as triple points, intergranular orientation mismatches, engineered inclusions and voids, and dynamic development of connections between voids are all part of our current work. This presentation will detail the results to date.

\(^1\)This work was funded through the LANL LDRD Program, Project 20060021DR.

9:45AM L2.00008 Deformation regimes in shocked nanocrystals: experiments and simulations\(^1\), Y.M. WANG, E. BRINGA, A. CARO, M. VICTORIA, J. MCGANEY, J. HAWRELIAK, R. SMITH, B. REMINGTON, H. LORENZANA, Lawrence Livermore National Laboratory, Livermore, M. MEYERS, H. JARMAKANI, UC San Diego — Transmission electron microscopy (TEM) of shocked nc samples shows dislocations for pure Ni with grain sizes above 30 nm grain, even at 70 GPa, which is more than twice the twinning threshold for shock-twinning in polycrystalline Ni. On the other hand, new experiments on NiW show a rich behavior, with twins only at 9 nm grain size and both dislocations and twins at grain sizes above 50 nm. We interpret this as due to the relatively low stacking fault energy (SFE) of NiW. A semi-analytical model is presented which is consistent with the experimental changes in the slip-twinning transition with grain size and stacking fault energy. MD of shock waves in nc Cu and nc Ni, which have very different SFE, are also consistent with the experimental results. The experiments, model and simulations provide a deformation map for nc under shock loading.

\(^1\)This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under contract No.W-7405-Eng-48, LDRD 04-ERD-021.

Wednesday, June 27, 2007 8:00AM - 10:00AM – Session L3 Phase Transitions II Fairmont Orchid Hotel Plaza I

8:00AM L3.00001 Effect of Pulse Duration on Polytetrafluoroethylene Shocked Above the Crystalline Phase II–III Transition, ERIC N. BROWN, GEORGE T. GRAY III, PHILIP J. RAE, CARL P. TRUJILLO, Los Alamos National Laboratory, Materials Science and Technology Division, NEIL K. BOURNE, AWE, UK — We present an experimental study of crystalline structure evolution of polytetrafluoroethylene (PTFE) due to pressure-induced phase transitions in a semi-crystalline polymer using soft-recovery, shock-loading techniques coupled with mechanical and chemical post-shock analysis. Gas-launched, plate impact experiments have been performed on pedigreed PTFE 7C, mounted in momentum-trapped, shock assemblies, with impact pressures above and below the phase II to phase III crystalline transition. Below the phase transition only subtle changes were observed in the crystallinity, microstructure, and mechanical response of PTFE. Shock loading of PTFE 7C above the phase II–III transition was seen to cause both an increase in crystallinity from 38% to ~53% (by Differential Scanning Calorimetry, DSC) and a finer crystalline microstructure, and changed the yield and flow stress behavior. We particularly focus on the effect of pulse duration on the microstructure evolution.

8:15AM L3.00002 Phase transformation kinetics - equilibrium and metastable conditions, MARINA BASTEA\(^1\), S. BASTEJ, J. REAUGH, D. REISMAN, Lawrence Livermore National Laboratory — The kinetics of first order phase transformations has been a topic of great experimental and theoretical interest. The development of new high pressure techniques has brought new perspectives on this problem and new insights on long-standing scientific puzzles e.g. the formation of natural diamond and the freezing of water. Dynamic compression experiments afford the study of equilibrium and non-equilibrium processes occurring on very short time-scales - \(10^{-12}\) to \(10^{-6}\) s, which are otherwise difficult to investigate with most traditional static high pressure techniques. I will discuss results on the freezing of water and diamond formation along quasi-adiabatic high pressure paths. For water the emphasis will be on dynamic features resembling Van der Waals loops while for carbon I will present results on diamond formation from different initial condition states. Both systems exhibit a large metastability range. A comparison with near-equilibrium phase transformations in other materials will also be included. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

8:30AM L3.00003 Kinetics of Phase Transition Under Tailored Dynamic Compression, JEFFREY H. NGUYEN, Lawrence Livermore National Laboratory, DANIEL ORLIKOWSKI, J. REED PATTERSON, L. PETER MARTIN, NEIL C. HOLMES, Lawrence Livermore National Laboratory — High Pressure-High Temperature phase boundaries are typically mapped out in static compression experiments where the kinetics of these phase transitions are not fully explored. Dynamic compression experiments, on the other hand, are traditionally limited to the principal Hugoniot or the principal quasi-isentrope. Recent advances of the functionally graded density impactor now allow us to explore the phase diagram of materials in previously inaccessible regions of the PVT phase diagram and at strain rates comparable to the time-scales of many phase transitions in metals and molecular liquids. We present here experiments exploring liquid-solid and solid-solid transitions on principal and “hot” quasi-isentropes. Our principal focus will be on the liquid-solid transition in water, but we will also discuss other solid-solid transitions in metals as appropriate. These phase transitions have been characterized with changes in both the particle velocity and optical properties. The kinetics of the water-ice transition will be discussed in terms of changes in the optical properties in addition to the time evolution of the ice volume fraction during the transition. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

8:45AM L3.00004 Experimental and computational investigation of the shock melting properties of diamond\(^1\), MARCUS KNUDSON, MICHAEL DESJARLAIS, RAYMOND LEMKE, Sandia National Labs — The shock melting of diamond has gained interest of late due to its possible use as an ablative material in inertial confinement fusion capsules. Recently, experiments utilizing the flyer plate capability at the Sandia Z accelerator were performed to determine the Hugoniot and the shock melting properties of polycrystalline diamond. Composite aluminum/copper flyer plates were used to shock load diamond samples to pressures ranging from 5 to 14 Mbar. Multiple samples and fast diagnostics provided Hugoniot measurements with roughly 1 percent accuracy in density. Furthermore, measurements of the release behavior may provide direct indication of the extent of the coexistence region on the Hugoniot. These high precision Hugoniot and release measurements at multi-Mbar pressures allow for high fidelity comparisons with recent quantum molecular dynamics calculations, and provide insight into the shock melting of diamond.

\(^1\)Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL850000
9:00AM L3.00005 Dynamic compression of diamond across the melt transition\textsuperscript{1}. PETER CELLIERS, Lawrence Livermore National Laboratory — The past two years have seen dramatic improvements in dynamic compression experiments on diamond using laser-induced compression methods. We will present an overview of our current experimental understanding of the phase-diagram and equation of state of high pressure carbon. We have carried out: (i) measurements of the shock Hugoniot up to 3600 GPa; and, (ii) measurements of the shock front temperature along the Hugoniot that show a clear slope discontinuity when the Hugoniot enters the solid-liquid coexistence region providing the first direct observation of the pressure-temperature locus along the melt curve between 850-1100 GPa. Comparison with recent quantum molecular dynamics calculations shows better agreement than with previous models. In addition, we have observed a rate-dependent elastic limit ranging between 60 and 200 GPa. From these experiments we have been able to extract a wide variety of thermodynamic quantities, including the latent heat of fusion, the volume discontinuity at melt and the specific heat at very high pressures. In collaboration with J.H. Eggert, D.K. Bradley, A.A. Correa, E.F. Schwager, D.G. Hicks, R.F. Smith, R.S. McWilliams, and G.W. Collins of LLNL; T.R. Boehly and J.E. Miller of the University of Rochester.

\textsuperscript{1}This work was performed under the auspices of the U. S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No.W-7405-Eng-48.

9:30AM L3.00006 Multiphase equation of state of Carbon from first principles simulations and applications to shock wave experiments and design\textsuperscript{1}. ALFREDO A. CORREA, Lawrence Livermore National Laboratory and Physics Department, University of California at Berkeley — Hydrodynamic and finite element simulations are of primary importance in the current point design of the Ignition capsules for fusion at the National Ignition Facility. In this lecture we present the design of the capsules as a two-temperature two-phase mix of solid and liquid carbon, and describe recent measurements of the shock Hugoniot up to 3600 GPa. We demonstrate the pressure-temperature locus along the melt curve between 850-1100 GPa and show that the pressure-temperature discontinuity is consistent with the predicted slope discontinuity. We also discuss the possibility of shock-induced melting in the capsules at the National Ignition Facility. In collaboration with J.H. Eggert, D.K. Bradley, A.A. Correa, E.F. Schwager, D.G. Hicks, R.F. Smith, R.S. McWilliams, and G.W. Collins of LLNL; T.R. Boehly and J.E. Miller of the University of Rochester.

\textsuperscript{1}This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

Wednesday, July 27, 2007 8:00AM - 10:00AM

Session L4 Continuum and Multiscale Modeling II Fairmont Orchid Hotel Plaza II

8:00AM L4.00001 Mesoscale and Continuum Calculations of Wave Profiles for Shock-Loaded Granular Ceramics\textsuperscript{1} . TRACY VOGLER, Sandia National Laboratories, JOHN BORG, Marquette University — A significant challenge in the multi-scale modeling approach is the validation of simulations performed at the various length scales considered. Recently, mesoscale modeling of the compaction of granular ceramics has been performed as part of a multiscale modeling approach. Through small adjustments to the model parameters, good agreement between the Hugoniot response for the experiments and simulations was obtained. Here, we evaluate the performance of the mesoscale model in predicting experimental velocity histories obtained with VISAR. In particular, we explore its ability to capture correctly the process of wave attenuation. For comparison, we will also examine the ability of continuum models such as the P-alpha and P-lambda models to correctly predict the wave profiles. The consideration of attenuating waves provides a means of validation not previously considered for these mesoscale simulations.

\textsuperscript{1}Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

8:15AM L4.00002 2D Mesoscale Simulations of Projectile Penetration into Sand . R.D. TEETER, S.K. DWIVEDI, C.W. FELICE, Y.M. GUPTA, Institute for Shock Physics, Washington State University — Physical Phenomena governing projectile instabilities during penetration of granular media (e.g. sand) are not well understood. To gain insight into projectile – granular media interactions, 2-D mesoscale simulations were performed to examine projectile penetration into sand targets with explicit representation of sand grains and representative porosities. The computational procedure used to generate a mesoscale representation of a sand target is presented with emphasis on an energy minimization technique for grain placement and modified Voronoi tessellations to enforce desired grain size and geometry. Simulated sand targets are shown to reproduce grain size distributions and porosities as large as 30% in close agreement with input parameters. Further, initial results from 2D mesoscale simulations, using the ISP-TROTP code, of normal impact of ogive shaped impactors at 0.5 km/s, 1.0 km/s, and 1.5 km/s impact velocities show that heterogeneous deformation in a frictionless granular media can cause deviation of projectile motion from normal direction indicating projectile instability during penetration. Efforts to achieve an improved description of granular media are underway. Work supported by DOE and AFOSR.

8:30AM L4.00003 Determination of simple constitutive models for DEDF glass using penetration-velocity data from ballistic experiments. GORDON JOHNSON, TIMOTHY HOLMQUIST, Network Computing Services Inc. — Constitutive models for brittle materials such as glass can be very complex as they are dependent on strains, strain rates, pressures, temperatures, damage and other parameters. There may also be significant (pressure-dependent) strength after failure such that the constitutive response is much different for intact material and failed material. A great number of laboratory tests are required to develop a comprehensive constitutive model. Another approach is to develop simple models using penetration-velocity data obtained from ballistic experiments. Here, various functional forms of simple models (with a limited number of constants) are used to (computationally) match the penetration velocity over a range of impact velocities. This allows for the determination of the most important parameters and it provides an approximation of the stresses that occur during penetration. This paper presents constitutive models for high-density DEDF glass. They are based on penetration-velocity data reported by Behner et al. (Proceedings of the 22\textsuperscript{nd} International Symposium on Ballistics, Vancouver BC, Canada, November 2005) for gold rods impacting DEDF glass at impact velocities from 400 to 2500 m/s.

8:45AM L4.00004 Multiscale Modeling of Shocked Ceramics, RUQIANG FENG, JIANBIN ZHU, University of Nebraska-Lincoln — Under shock compression, polycrystalline ceramics may undergo mesoscopically heterogeneous inelastic deformation via transgranular slip or twinning in some grains. Although polycrystal modeling, which accounts for crystal anisotropies and grain-to-grain topological variations and permits implementation of crystal plasticity models of interest, may be used to analyze such a deformation, the size affordable is too small to run wave propagation simulations from first principles. Therefore, we have developed a multiscale modeling technique, in which a Voronoi polycrystal is embedded in a homogeneous matrix of the size proper for simulating the experiment. The polycrystal model considers nonlinear crystal elasticity and microplasticity by limited slip systems. The matrix model uses the mean stress response predicted by elastic polycrystal simulation and a strength model combining the Drucker-Prager plasticity with a prescribed limiting strength. Two parametric optimizations are pursued iteratively. One is to optimize the material parameters to match the simulated wave profile with the measurement. The other is to optimize the polycrystal parameters to match the experimental velocity histories obtained with VISAR. In particular, we explore its ability to capture correctly the process of wave attenuation. For comparison, we will also examine the ability of continuum models such as the P-alpha and P-lambda models to correctly predict the wave profiles. The consideration of attenuating waves provides a means of validation not previously considered for these mesoscale simulations.
9:15AM L5.00005 Time-Resolved Optical Measurements of Detonation and Combustion Products
JOEL CARNEY, JOHN WILKINSON, JAMES LIGHTSTONE, Indian Head Division, NSWC — This presentation exhibits our initial attempts at measuring detonation and combustion products using time-resolved absorption spectroscopy. Transient species in the post-detonation combustion environment of a fuel-rich explosive event include emissive and non-emissive products ranging in size from atomic to macroscopic. The time-resolved concentrations of emissive and non-emissive species relate to the overall efficiency of the detonation. Recently, our group has used streak-camera based time-resolved emission spectroscopy to directly measure the relative concentrations of emissive species in a detonation environment. To relate measured emission intensities to a total species concentration vs. time in the environment following a detonation, the ratio of emissive and non-emissive species need to be estimated. In this presentation, we compare concentrations of post-detonation combustion transient species (aluminum and aluminum monoxide) measured by time-resolved emission spectroscopy and time-resolved absorption spectroscopy. Pressed samples of PETN and aluminum are used as controlled, fuel-rich explosive mixtures. The absorption measurements are directly proportional to the transient concentration and serve to scale the relative emission measurement to the total (emissive + non-emissive) concentration.

9:30AM L5.00006 Characterization and use of a CO\textsubscript{2} infrared laser for ignition of explosives
JEREMY MONAT, NSWC Indian Head, EDWARD TERSINE, BRENT MORGAN, NSWC Indian Head, PETER OSTROWSKI, Energetic Materials Technology — This abstract reports on the characterization and use of a 200W, 10.6 \mu\text{m} CO\textsubscript{2} laser for nonresonant ignition of explosives. To characterize the laser, we measured its risetime with a diode whose response time is approximately 125 ns. We also measured the beam’s spatial profile with a scanning pinhole setup. Next, we used the laser for testing of explosives for fundamental research and CAD/PAD (cartridge-actuated devices/propellant actuated devices) applications. Specifically, we determined energy-to-ignition values for TNT (2,4,6-trinitrotoluene) and the novel primary KDNP (4,6-dinitro-7-hydroxybenzofuroxan). Ignition was judged to begin at first light, which occurs when the laser-induced reaction first emits light as detected by a visible photodiode. To determine the energy to ignition accurately, we corrected the laser power for reflections. We used a high-speed camera to monitor the reaction progress from ignition to explosive consumption.

9:45AM L5.00007 Time-Resolved Spectroscopic Measurements of Aluminum Oxidation in a Laser Ablation Event
JAMES LIGHTSTONE, JOEL CARNEY, Indian Head Division, Naval Surface Warfare Center — Laser ablation of an aluminum sheet is used to create a high pressure and temperature environment for the investigation of aluminum (Al) oxidation. High energy pulsed lasers are used to initiate the ablation and to probe oxidation products in the expanding plume as a function of time and space. Emission, absorption, and scattering spectroscopies are used to deduce information on the observed reaction pathways, species concentrations, and internal energies. Emission measurements using a streak camera with 0.1 nm spectral resolution exhibit the line profiles of atomic Al and aluminum monoxide (AlO), which are sensitive to excited state populations and internal energy distributions. Analogous ground state information is recorded using absorption (laser induced fluorescence) spectroscopy. In general, comparable emission and absorption results often display a level of equilibrium within the expansion. Results from these studies will be presented along with progress toward adapting optical scattering (Raman) spectroscopies to identify additional aluminum oxide species formed in the ablation plume. The application of the spectroscopic techniques presented toward the measurement of a dynamic chemical process such as a detonating fuel-rich explosive formulation will also be discussed.

Wednesday, June 27, 2007 8:00AM - 10:00AM
Session L6 Shock Initiation I Fairmont Orchid Hotel Promenade I/II

8:00AM L6.00001 Shock Initiation Experiments on PBX 9501 Explosive at Pressures Below 3 GPa with Associated Ignition and Growth Modeling
STEVEN K. CHIDESTER, DARLA G. THOMPSON, KEVIN S. VANDERSALL, DEANNE J. IDAR, CRAIG M. TARVER, FRANK GARCIA, PAUL A. URTIEW, LAWRENCE LIVERMORE NATIONAL LABORATORY — Shock initiation experiments on the explosive PBX 9501 (95% HMX, 2.5% estane, and 2.5% nitroplasticizer by weight) were performed at pressures below 3 GPa to obtain in-situ pressure gauge data, run-distance-to-detonation thresholds, and Ignition and Growth modeling parameters. A 101 mm diameter propellant driven gas gun was utilized to initiate the PBX 9501 explosive with manganin piezoresistive pressure gauge packages placed between sample slices. The run-distance-to-detonation points on the Pop-plot for these experiments showed agreement with previously published data and Ignition and Growth modeling parameters were obtained with a good fit to the experimental data. This parameter set will allow accurate code predictions to be calculated for safety scenarios in the low-pressure regime (below 3 GPa) involving PBX 9501 explosive. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

8:15AM L6.00002 Shock Initiation Experiments on the HMX Based Explosives LX-07 and LX-10 with Associated Ignition and Growth Modeling
KEVIN S. VANDERSALL, CRAIG M. TARVER, FRANK GARCIA, PAUL A. URTIEW, STEVEN K. CHIDESTER, Lawrence Livermore National Laboratory — Shock initiation experiments on the HMX based explosives LX-10 (95% HMX, 5% Viton by weight) and LX-07 (90% HMX, 10% Viton by weight) were performed to obtain in-situ pressure gauge data, run-distance-to-detonation thresholds, and Ignition and Growth modeling parameters. A 101 mm diameter propellant driven gas gun was utilized to initiate the explosive samples with manganin piezoresistive pressure gauge packages placed between sample slices. The run-distance-to-detonation points on the Pop-plot for these experiments and prior experiments on another HMX based explosive LX-04 (85% HMX, 15% Viton by weight) will be shown, discussed, and compared as a function of the binder content. This parameter set will provide additional information to ensure accurate code predictions for safety scenarios involving HMX explosives with different percent binder content additions. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

8:30AM L6.00003 Extended run distance measurements of shock initiation in PBX 9502
RICK GUSTAVSEN, STEVE SHEFFIELD, RICK ALCÓN, Los Alamos National Laboratory — We have completed a series shock initiation experiments on two lots of PBX 9502 (95 weight % TATB, 5 weight % Kel-F 800 binder). One PBX 9502 lot contained few fine particles (10 weight % < 20 microns) while the second lot contained many fines (39 weight % < 20 microns). Large, 71 mm diameter PBX 9502 samples were used and input pressures were 7.5 – 0.5 GPa resulting in run distances to detonation of 25 – 35 mm. These results extend previous work [J. Appl. Phys. 99, 114907 (2006)] in which we used 43 mm diameter samples, input pressures > 10.5 GPa, and measured run distances < 15 mm. Buildup to detonation was measured using embedded magnetic particle velocity gauges. An unusual feature of the work was the use of metallic impactors (316 stainless steel) in combination with magnetic gauges. It has previously been assumed that conducting impactors would badly perturb the magnetic gauge measurements; however, we observed no ill effects other than a nearly constant baseline shift of ≈ 10%. Results include reaction rates at the impact surface and distance to detonation vs. initial pressure. No lot to lot differences in initiation behavior were observed.

1Supported by the US DOE under contract DE-AC52-06NA25396.
8:45AM L6.00004 Shock Reactivity of Non-Porous Mixtures of Manganese and Sulfur . FRANCOIS-XAVIER JETTE, SAMUEL GOROSHIN, ANDREW HIGGINS, McGill University, SHOCK WAVE PHYSICS GROUP TEAM — Stoichiometric mixtures of manganese powder and sulfur were melt-cast into solid pellets in order to study the mechanism of shock-enhanced reactivity in non-porous heterogeneous mixtures. This mixture was selected due to the large exothermic heat release of the manganese-sulfur reaction (214 kJ/mol), which causes the reaction to be self-sustaining once initiated. The test samples were placed in planar recovery ampoules and a strong shock was delivered via the detonation of a charge of amine-sensitized nitromethane. Various shock strengths were achieved by placing different thicknesses of PMMA attenuator between the explosive charge and the ampoule. The results confirmed that shock-induced reactions can be produced in the absence of porosity. Indeed, the critical shock pressure that caused ignition of the mixture in the ampoule was found to be in the range 2.2 - 3.8 GPa (pressures were estimated using LS-DYNA simulations). In the cases where the shock was too weak to cause ignition in the ampoule, the sample was extracted and its ignition temperature was determined using a differential thermal analyzer.

9:00AM L6.00005 Time-Resolved Temperature Measurements of Shock Initiation in a Manganese-Sulfur Mixture . FRANCOIS-XAVIER JETTE, SAMUEL GOROSHIN, ANDREW HIGGINS, McGill University, SHOCK WAVE PHYSICS GROUP TEAM — Previous tests carried out in planar recovery capsules showed that strong (3-8 GPa) shock waves, generated by a charge of amine-sensitized nitromethane and attenuated by a PMMA layer, can initiate reactions in non-porous stoichiometric mixtures of manganese and sulfur. The current study focused on the onset of these reactions using time-resolved temperature measurements. A photomultiplier-based two-color pyrometer was used to record sample temperatures shortly after the passage of the shock while a thermocouple was used to record temperatures over longer time scales. An experimental complication encountered when studying shock-induced reactions in porous energetic materials using pyrometry, i.e. intense light due to large localized heating, can be mostly eliminated if a non-porous sample is studied. Further, in order to increase the reliability of the pyrometry results, the reactive test mixture (Mn+S) was chosen to have a high heat of reaction (214 kJ/mol) and thus a high reaction temperature, and baseline tests were performed with inert melt-cast mixtures of WS2 and sulfur.

9:15AM L6.00006 ABSTRACTWithDRAWN —

9:30AM L6.00007 Observations of shock-induced partial reactions in high explosive . SHIRO KUBOTA, YUJI OGATA, YUJI WADA, TEI SABURI, National Institute of Advanced Industrial Science and Technology. KUNIHIKO NAGAYAMA, Department of Aeronautics and Astronautics, Faculty of Engineering, Kyushu University — The high speed photography, pressure measurements and numerical simulation of gap test of the high explosive have been carried out. The height of donor is 50 mm and acceptor is 40 mm with 26 mm inner diameter. When the gap length is 23 mm or large, the sympathetic detonation was not confirmed. Although the detonation does not occur, the gas expansion from the acceptor appears as the results of remarkable decomposition if the gap length approaches 23 mm. Those phenomena are very important on the point of view of the safety engineering. Finally, the parameters of initiation model which could reproduce the behaviors of high explosive around the critical condition were constructed.

9:45AM L6.00008 Large Area and Short Pulsed Shock Initiation of A TATB/HMX Mixed Explosive . GUIJI WANG, CHENGWEI SUN, JUN CHEN, CANGLI LIU, FULI TAN, NING ZHANG, Institute of Fluid Physics, Chinese Academy of Engineering Physics — The large area and short pulsed shock initiation experiment on a plastic bonded mixed explosive of TATB(80%) and HMX(15%) has been performed with an electric gun where a mylar flyer of 19mm in diameter and 0.05~0.30mm in thickness is launched by an electrically exploding metallic bridge foil. The cylindrical explosive specimens (916mm × 8mm in size) were initiated by the mylar flyers in thickness of 0.07~0.20mm, which induced shock pressure in specimen was duration ranging 0.029~0.109µs. The experimental data were treated with the DRM(Delayed Robbins-Monro) procedure and to provide the threshold of shock pressure P 13.73~5.23GPa. The shock initiation criterion of the explosive specimen is (P/GPa)1/4.151(τ/µs) = 2.63. In addition, the 30° wedged specimen was tested and the shock to detonation transition (SDT) process emerging on its inclined surface was diagnosed with a device consisting of multiple optical fiber probe, optoelectronic transducer and digital oscilloscope. The P0P plot of the explosive has been gained from above SDT data.

2This work is supported by NNSFC(10472108) and Key Foundation of CAEP(200420101).

Wednesday, June 27, 2007 8:00AM - 9:45AM –

Session L7 Inelastic Deformation-Aluminum

Fairmont Orchid Hotel Promenade III

8:00AM L7.00001 1D Continuum and 2D Mesoscale Simulations of Plate Impact Spall Experiments in 6061-T6 Aluminum . S.K. DWIVEDI, J.N. JOHNSON, Y.M. GUPTA, Institute for Shock Physics, Washington State University — A comprehensive study has been initiated to understand the spallation of 6061-T6 aluminum in plate impact experiments, and to relate the features in pull-back velocity profile to material damage. Plate impact spall experiments at three stress levels 4.1 GPa, 13.7 GPa, and 21 GPa with two sample thicknesses at 4.1 GPa were simulated using Johnson’s void growth and coalescence model in a 1D wave code COPS. The results show that the model allows determination of a common set of parameters (with some tolerance) that simulates pull-back velocity profile for all the four experiments. More importantly, the maximum tensile stress at the spall plane is higher than the spall threshold stress calculated from the pull-back velocity and does not increase with thickness reduction. These phenomena are under further study through 2D mesoscale simulations which are known to predict quasi-elastic unloading without shear modulus degradation as needed in 1D COPS. Results from 1D COPS and 2D mesoscale simulations will be compared to highlight the material phenomena. Work supported by DOE.

8:15AM L7.00002 Dynamic Response of 5083-H131 Aluminum Alloy . JOHN BOTELER, NSWC-Indian Head, DATTATRAYA DANDEKAR, Army Research Laboratory — The material response of 5083-H131 aluminum alloy subjected to dynamic loading has been investigated. In the work reported here we examine the spall strength, Hugoniot EOS, and Hugoniot Elastic Limit (HEL) over the stress range 1.5-8.0 GPa. Measurement of these dynamic properties provide hydrocode models with critical information required for accurate modeling of material response to intense loading. Experiments were performed on the Army Research Laboratory 102 mm bore single-stage light gas gun. Impact conditions were uniaxial and planar to within 1 mrad of tilt. VISAR was used to record particle velocity histories with 0.5 ns temporal resolution. The shock Hugoniot for 5083-H131 is extrapolated to 50 GPa and compared to the previous high pressure results of Hauver (1973). The dynamic response including HEL and spall strength of 5083-H131 is compared to other commonly used aluminum alloys.
8:30AM L7.00003 2D Mesoscale Simulations of Quasielastic Reloading and Unloading in Shock Compressed Aluminum\textsuperscript{1}, S.K. DWIVEDI, Institute for Shock Physics, Washington State University — 2D mesoscale simulations of planar shock compression, followed by either reloading or unloading, are presented that predict quasi-elastic (QE) response observed experimentally in shocked polycrystalline aluminum. The representative volume element (RVE) of the plate impact experiments included a realistic representation of a grain ensemble with apparent heterogeneities in the polycrystalline sample. Simulations were carried out using a 2D updated Lagrangian finite element code ISP-TROTP incorporating elastic-plastic deformation in grain interior and contact/cohesive methodology to analyze finite strength grain boundaries. Local heterogeneous response was quantified by calculating appropriate material variables along in-situ Lagrangian tracer lines and comparing the temporal variation of their mean values with results from 2D continuum simulations. Simulations were carried out by varying a large number of individual heterogeneities to predict QE response on reloading and unloading from shock state. The heterogeneities important for simulating the QE response identified from these simulations were: hardened grain boundaries, hard inclusions, and micro-porosity. It is shown that the shock-deformed state of polycrystalline aluminum in the presence of these effects is strongly heterogeneous with considerable variations in lateral stresses. This distributed stress state unloads the shear stress from flow stress causing QE response on reloading as well as unloading. The simulated velocity profiles and calculated shear strength and shear stresses for a representative reloading and unloading experimental configuration were found to agree well with the reported experimental data. Work supported by DOE.

\textsuperscript{1}Collaborations with Dr. J.R. Asay and Prof. Y.M. Gupta are acknowledged.

9:00AM L7.00004 Laser-Induced Spall of Aluminum and Aluminum Alloys at High Strain Rates, DOUGLAS DALTON, JONATHAN BREWER\textsuperscript{1}, AARON BERNSTEIN, WILL GRIGSBY, DESPINA MILATHIANAKI, EVAN JACKSON, University of Texas-Austin, RICHARD ADAMS, PATRICK RAMBO, JENS SCHWARZ, AARON EDENS, MATTHIAS GEISSEL, IAN SMITH, Sandia National Laboratory, ERIC TALEFF, TODD DITMIRE, University of Texas-Austin — We report on laser-induced spall experiments aimed at studying how a material’s microstructure affects the tensile fracture characteristics at high strain rates (>10\textsuperscript{10} s\textsuperscript{-1}). We used the Z-Beamlet Laser at Sandia National Laboratory to drive shocks and to measure the spall strength of aluminum targets with various microstructures. The targets were recrystallized, high-purity aluminum (Al-HP RX), recrystallized aluminum + 3 wt.% magnesium (Al-3Mg RX), and cold-worked aluminum + 3 wt.% magnesium (Al-3Mg CW). The Al-3Mg RX and Al-3Mg CW are used to explore the role that solid-solution alloying and cold-working have on the spall strength. Using a VISAR and sample recovery techniques, we are able to measure spall strength and failure morphology in these targets simultaneously. We find that the spall strength is highest for Al-HP RX. Analysis reveals that material grain size plays a vital role in the fracture morphology and spall strength results.

9:30AM L7.00006 Shock Consolidation of Nanocrystalline Aluminum Powders for Bulk Component Formation, DAVID A. FREDENBURG, Georgia Institute of Technology, TRACY VOGLER, Sandia National Labs, CHRISTOPHER SALDANA, Purdue University, NARESH THADHANI, Georgia Institute of Technology — Shock compression is used to consolidate micron-size nanocrystalline metal particles formed from Al-6061 T6 stock through frequency modulated severe plastic deformation (SPD) machining methods. Compaction characteristics are developed in the quasi-static and dynamic shock regime. Shock recovery experiments are performed to determine the degree of densification, and the microstructure and mechanical properties of compacts following shock compression. At lower impact velocities compacts show slight increase in crystallite size and reduction in residual strain for bulk compacts reaching 85-92% theoretical density, with microstructures revealing a lack of mechanical bonding between neighboring particles. At higher impact velocity of 650 m/s compacts reach 95-96% theoretical density. Mesoscale simulations using real microstructures obtained from powder compacts are performed to examine the shock propagation characteristics through the simulated compacts and determine the effect of particle morphology on compaction characteristics. Simulations will also aid in design of the compaction experiments to ensure fabrication of bulk compacts with retention of nanocrystalline grain structure.

Wednesday, June 27, 2007 10:30AM - 12:45PM – Session M2 First Principles and Molecular Dynamics Calculations III Fairmont Orchid Hotel Amphitheater

10:30AM M2.00001 Molecular Dynamics Studies of Thermal Induced Chemistry in TATB\textsuperscript{1}, JASON QUENNEVILLE, TIMOTHY GERMANN, Los Alamos National Laboratory — A reactive force field (ReaxFF\textsuperscript{2}) is used with molecular dynamics to probe the chemistry induced by intense heating (accelerated ‘cook-off’) of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Large-system simulations are desired for TATB because of the high degree of carbon clustering expected in this material. Using small, 800-atom, simulations, we will show the reaction rate as a function of temperature and density as well as the time evolution of reaction products. A larger simulation (with 14,000 atoms) will illustrate the effect of reaction products in TATB crystals under various thermal and shock conditions.

\textsuperscript{1}This work was performed at Los Alamos National Laboratory (LANL) under U.S. Department of Energy contract DE-AC52-06NA25396.

10:45AM M2.00002 Initial steps of condensate-phase decomposition of TATB from reactive molecular dynamics\textsuperscript{1}, HYUNJUN KIM, SERGEY ZYBIN, ADRI VAN DUIJN, WILLIAM GODDARD, California Institute of Technology — The initial steps of condensate-phase decomposition of TATB high explosive have been investigated by molecular dynamics method using ReaxFF reactive force field parameterized from the first-principles calculations. We study the dependence of primary and secondary reaction kinetics on the initial temperature and density both in pure crystal and in presence of various defects such as voids and inclusions. We found that at lower temperature the primary decomposition steps mainly involve intramolecular hydrogen transfer followed by the formation of water molecules while at higher temperatures the homolytic cleavage of N-NO\textsubscript{2} bond can appear, providing a temperature-dependent effect on the decomposition pathway. Besides, we also observe the formation of carbonaceous clusters during thermal and shock induced decomposition in TATB that initially capture large amount of the oxygen and nitrogen atoms delaying secondary reactions of small molecules and further transformation of the cluster into carbon soot. We analyze the primary and secondary reaction mechanisms as well as the evolution of decomposition products in TATB crystals under various thermal and shock conditions.

\textsuperscript{1}Acknowledgements: supported by ARO and ONR grants.
11:00AM M2.00003 Atomicistic Studies of Energetic Materials Under Shock Wave Loading

THOMAS SEWELL, Theoretical Division, Los Alamos — We have recently undertaken non-equilibrium molecular dynamics studies to aid our understanding of dynamical processes in the high explosives HMX and RDX, in particular the inelastic, anisotropic response of crystals of those materials subjected to quasi-static and shock loading. The overarching goal of this work is to provide information that can serve as a foundation in basic science for the formulation of improved mesoscale constitutive models for the constituent materials in selected energetic formulations. The medium-term scientific challenge to this larger objective is to carefully identify, characterize, and quantify the dominant mechanisms of localization and dissipation in such materials, under a variety of prescribed quasi-static and dynamic loading scenarios that lead to inelastic deformation of the crystals. The focus of the present talk will be the unreactive shock response of structurally perfect, but properly thermalized, HMX and RDX crystals; and shock localization in defective RDX crystals. Effort will be made to present information of interest to the shock physics, materials science, and chemical dynamics/spectroscopy communities.

11:30AM M2.00004 Shear-strain Sensitivity of Energetic Crystals and the Origin of Hot-spots

MAJJA KUKLJA1, Division of Materials Research, National Science Foundation, SERGEY RASHKEEV2, Center for Advanced Modeling & Simulation, Idaho National Laboratory — Simulation of shear-induced chemical reactions of decomposition of crystalline FOX-7 and TATB is performed by means of Density Functional Theory and First Principles Molecular Dynamics. It is shown that the shear-strain deformation plays a crucial role in defining the sensitivity of explosive crystals to initiation and strongly depends on the shape of crystalline lattice constituting the material. Energetic barriers for FOX-7 decomposition are found to decrease due to shear while those for TATB are not affected by this deformation. We discuss possible mechanisms of chemistry in hot spots, associated with the local shear-strain deformation. This work made possible to provide specific recommendations for synthesis of insensitive energetic materials.

11:45AM M2.00005 Molecular dynamics simulation of the shock-induced wurtzite-to-rocksalt transition in CdSe and CdS

AIDAN THOMPSON, MARCUS KNUDSON, Sandia National Laboratories — The shock-induced wurtzite-to-rocksalt structural transformation is studied using large-scale molecular dynamics simulation. The primary goal is to understand the atomistic mechanisms underlying the interesting transformation observed in the case of cadmium sulfide [M. D. Knudson and Y. M. Gupta, J. Appl. Phys, v. 91, p. 9561, 2002]. Since the mechanical and structural properties of cadmium selenide are similar to those of cadmium sulfide, as a first step multi-million atom shock propagation simulations have been carried out in CdSe using the Rabani force field, which has been shown to correctly describe the important bulk phases of CdSe, as well as the wurtzite-to-rocksalt deformation. As a next step a force field for CdS will be developed to enable comparison of similar shock propagation simulations with experiments.

12:00PM M2.00006 Molecular Dynamics Simulation of TATB-like Explosive

VLADIMIR DREMOV, ILYA DERBENEV, ALEXEY KARÁVAEE, RFNC-VNIITF, LAURENT SOULARD, CEA/DAM — A modification of REBO potential has been proposed for the molecular dynamics simulation of a TATB-like condensed explosive whose molecule initially consists of four different atoms. TATB-like means bulk properties of initial state and parameters at CJ point similar to those of real TATB. Parameters of the potential are subdivided into two groups that are responsible for CJ parameters and reaction zone width. The possibility of formation of intermediate detonation products allows variation of reaction zone characteristics without changing CJ parameters. Provided are a number of test MD calculations on the thermodynamic properties of both the original explosive and detonation products, parameters at CJ point, reactions rates and reaction zone width as dependent upon the potential parameters as well as the evaluation of critical diameter. Mechanism of the detonation initiation proper to heterogeneous explosives has been investigated.

12:15PM M2.00007 Elastic and thermodynamic properties of post-perovskite MgSiO3, from first-principles calculations

LIU ZI-JIANG, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, P. O. Box 919-102, China Academy of Engineering Physics, Mianya — The elastic and thermodynamic properties of post-perovskite MgSiO3 polymorph are investigated at high pressures and temperatures using the plane wave pseudopotential method within the local density approximation. This phase may be the most abundant mineral in the D'' region. It is found that the post-perovskite phase has similar bulk modulus and larger shear modulus than perovskite at relevant pressures. The athermal elastic constant tensor of post-perovskite MgSiO3 are calculated as a function of pressure up to 200 GPa. The calculated results are in acceptable agreement with other predictions over the pressure regime studied. The thermodynamic properties of post-perovskite MgSiO3 polymorph are predicted using the quasi-harmonic Debye model; the heat capacity and thermal expansion coefficient accord with the other calculations at high pressures and temperatures.

12:30PM M2.00008 Predicting noncovalent interactions with nonlocal density functional theory

JOE HOOPER, FRANK ZERILLI, Naval Surface Warfare Center, Indian Head Division, NIC ROMERO, BETSY RICE, Army Research Laboratory — We report calculations using a new, nonlocal density functional which explicitly treats long-range van der Waals correlation in a nonempirical way. This method is designed to model complex electron interactions such as dispersion, an area where traditional DFT methods often perform poorly. The functional performs quite well for certain types of noncovalent bonding, producing energies within a few percent of high-level CCSD(T) and MP2 methods at a fraction of the calculation time. The nonlocal correlation scales appropriately under compression, reducing to accurate GGA results at intramolecular length scales. Intermolecular distances are generally overpredicted compared to coupled-cluster results; this is largely an artifact of the GGA exchange component, and can be improved by incorporating exact exchange. This new method appears to be quite promising for treating complex organic molecular crystals at a range of pressures.

Wednesday, June 27, 2007 10:30AM - 12:45PM
Session M3 Stress-Strength Measurements
Fairmont Orchid Hotel Plaza I

10:30AM M3.00001 Shear Strength Response of the Aluminium Alloy 6082-T6 During One-Dimensional Shock Loading

JOHN HARRIGAN, University of Aberdeen, JEREMY MILLETT, AWE, NEIL BOURNE, University of Manchester — The measurement of shear strength via the use of lateral stress gauges has been shown to be a viable technique in a number of materials. An experimental investigation on the intermediate-rate behaviour and shock response of the aluminium alloy, 6082-T6, is reported here. Results obtained using the lateral stress gauge technique show that the shear strength increases with impact stress. The lateral stress behind the shock front is seen to be relatively flat, unlike many other face-centred cubic metals and alloys, where a decrease in lateral stress indicates an increase in shear strength. This unusual response may be a reflection of the high stacking fault energy of aluminium and its alloys resulting in a reduction of the work hardening (i.e. increases in dislocation and/or twin density). Further plate impact results show that the Hugoniot of 6082-T6 is in effect identical to that of the more widely known 6061-T6. Split Hopkinson pressure bar results are used to provide a fuller picture of the rate-dependent behaviour of 6082-T6 over a range loading rates and conditions. Key words: shear strength, aluminium alloy, one-dimensional shock
10:45AM M3.00002 Constitutive Model Constants for Low Carbon Steels from Tension and Torsion Data1, NACHHATTER BRAR, University of Dayton Research Institute, Dayton, OH, VASANT JOSHI, Naval Surface Warfare Center, Indian Head, MD, BRYAN HARRIS, University of Dayton Research Institute — Low carbon C1010 steel is characterized under tension and torsion to determine Johnson-Cook (J-C) strength model constants. Constitutive model constants are required as input to computer codes to simulate projectile (fragment) impact on structural components made of this material. J-C model constants (A, B, n, C, and m) for the alloy are determined from tension and torsion stress-strain data. Tension tests are performed at a strain rate of \( \sim 1/s \) at room temperature. Tests at high strain rates are performed at high temperatures to 750°C. J-C strength model constants determined from these data: A=367 MPa, B=700 MPa, n=0.935, C=0.045, and m=0.643. Similar values for other low carbon steels (1006, 1008, and 1020) are compared. Torsion tests at quasi-static and high strain rates are performed at room and high temperatures. J-C model constants are evaluated from equivalent tensile stress-strain data obtained from torsion data using von Mises flow rule. These constants are compared to those determined from directly measured tensile data.

\[1\] Supported by the US Naval EOD Tech. Div., Indian Head, MD.

11:00AM M3.00003 Strength of materials in the diamond anvil cell to 1 Mbar. THOMAS DUFFY, Princeton University — The yield strength of materials at high pressure has diverse applications to interpretation of static and dynamic experiments, understanding mechanical performance, and constraining the rheology of planetary interiors. In recent years, diamond anvil cell techniques have been developed to measure lattice strain under non-hydrostatic loading using synchrotron X-rays. These studies constrain yield strength and provide insights into elastic moduli, equation of state, and texture development. Here we report results using this method to characterize the strength of a suite of metals (e.g., W, Re) and ceramics (e.g., B₄O, MgSiO₃) to pressures up to 1 Mbar. In general, strength increases with compression at a rate greater than the shear modulus, implying significant strain hardening under diamond cell loading. For W, the strength under static loading is comparable to that observed under dynamic quasi-isentropic loading. At pressures of 20-80 GPa, metals typically exhibit strengths of 1-3% of the shear modulus, \( G \). Strong coherent oxides possess yield strengths that range from 4-8% of \( G \). The consistency of strength trends across material classes suggests that reasonable empirical predictions of strength in the multimegabar pressure regime can now be made. Future advances can be expected to improve the capabilities of the diamond cell as a deformation device with the goal toward eventual direct determination of rheological properties at very high P-T conditions.

11:30AM M3.00004 Hydrocode Analysis of Lateral Stress Gauges in Shocked Tantalum, ERNEST HARRIS, RON WINTER, AWE — Experiments published by other workers on the resistance change of manganin stress gauges embedded in a lateral orientation in Tantalum targets have been analysed using an Adaptive Mesh Refinement Hydrocode. It was found that for four experiments the shape of the time profile of the computed lateral stress in the mounting layer closely matched the shape of the experimental lateral stress profiles. However, the calculated lateral stresses at the gauge location in the target material were significantly less than the stresses that would have been produced in the target if no gauge had been present. The perturbation caused by the gauge increased as the strength of the applied shock increased. When the perturbations are taken into account values of flow stress that are significantly smaller than those reported in the original research paper are derived. The work demonstrates that the lateral gauge technique can give valuable information on strength provided high resolution simulation is used to compensate for the perturbations caused by the gauges.

11:45AM M3.00005 Perturbations Caused by Lateral Stress Gauges, RON WINTER, ERNIE HARRIS, AWE, Aldermaston, UK — In principle, stress gauges mounted to measure lateral stresses in a shocked matrix allow the shear strength of the material to be determined. Interpreting the records from lateral stress gauges is hindered by the fact that the stress field in the insulating layer in which the gauges are mounted can differ significantly from the stress field that would be generated in the sample if no gauge were present. A series of high resolution Eulerian code calculations have been run which suggest that the stresses in the insulating layer vary with distance and time in a way that depends on the thickness of the layer, the shock strength, and the elastic and plastic properties of both the layer and the matrix. In particular, if the shock velocity in the matrix material is high the stress at a typical gauge position initially rises to a sharp peak then falls with time, but when the shock velocity in the matrix is low the stress rises relatively gradually throughout the time of interest. The shapes of the stress-time profiles predicted by the hydrocode compare well with the results of lateral gauge experiments on several different materials.

12:00PM M3.00006 Split Hopkinson Pressure Bar and Direct Impact Testing of Rohacell Foam, ELISAVET PALAMIDI, University of Manchester, JOHN HARRIGAN, University of Aberdeen, QINGMING LI, University of Manchester — Rohacell foam is a low density close-cell poly(methyacrylamide) rigid foam used as a core material in sandwich panels which are utilised in aircraft and marine constructions and in radiation applications. As such its dynamic properties are important. Two foam densities, Rohacell 51WF and 110 WF, have been tested at quasi-static and intermediate strain rates along their three principal directions. Typically, the foams have plateau strengths of 1 and 3 MPa in their strongest direction and corresponding densification strains of 0.66 and 0.6. Due to the low strength of the foams, the split Hopkinson pressure bar (SHPB) tests were carried out on low impedance PMMA bars. The propagation coefficient was determined experimentally to account for wave dispersion and attenuation in the bars. Wave separation was used to measure large strains. The foam properties appear broadly independent of strain rate. Direct impact tests were carried out to measure proximal and distal end forces at impact velocities of between 40 and 120 m.s⁻¹. With increasing impact velocity, the deformations are localized at a compaction front. The proximal stresses increase as predicted by the Rankine-Hugoniot conditions.

12:15PM M3.00007 Hopkinson Bar Studies of a PBX Simulant, DANIEL DRODGE, JOHN ADDISS, DAVID WILLIAMSON, WILLIAM PROUD, University of Cambridge — A Split Hopkinson Pressure Bar System was equipped with an environmental chamber for high and low temperature studies of a HTPB/sugar propellant simulator. Experiments were carried out, at a strain rate of \( \sim 1600\text{s}^{-1} \), to characterise the material response above and below the glass transition temperature. Other techniques were deployed, including high-speed photography with Digital Image Cross-Correlation analysis for flow visualisation, and a line-laser occlusion method, to determine the dynamic Poisson’s ratio. This paper outlines the current state of research and details the important observations to date.

12:30PM M3.00008 High-pressure Carbon Strength Model: first guess1, DANIEL ORLIKOWSKI, Lawrence Livermore National Laboratory, University of California — In support of National Ignition Facility experiments, there have been several sets of laser compression experiments performed on carbon. Our group has developed a simple model for carbon that can be used to predict the pressure dependence of the strength of carbon. In this model, the strength can be calculated, using robust density function theory (DFT), the equation of state (EOS) (A. Corea and L. Benedict) has also been performed. However, historically an adequate strength model is difficult to develop, due to a lack of data in general. Here, we give a simple interpretation of the experiments to develop a Steinberg-Guinan-like model based upon experimental observations and DFT calculations of the elastic moduli. We discuss this model and its use in particle velocity histories.

\[1\] This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract W-7405-Eng-48.

Wednesday, June 27, 2007 10:30AM - 1:00PM
Session M4 Geophysics and Planetary Physics Fairmont Orchid Hotel Plaza II
10:30AM M4.00001 The Deep Impact Oblique Impact Experiment. PETER H. SCHULTZ, Department of Geological Sciences, Brown University, Providence, RI 02912-1846 — The Deep Impact experiment represents a unique challenge. Without being able to see clearly the final crater, properties of the target requires comparing the ballistic ejecta with analytical and theoretical models for crater excavation. But the appropriate excavation model needs to be identified first. Consequently, each critical stage of cratering observed for the DI collision (initial coupling, late-stage ejection) is described and compared with a wide range of laboratory experimental results. The early-time flash and vapor plume rapidly evolve along the trajectory: an initial faint “first light” uprange from the projected point of impact; a fading source along the trajectory that moves downrange (~100-170m) over the next 0.125s after impact; gradual brightening over the next 0.62s; and then a sudden “flash” (saturated pixels) around 0.25s after the “first light.” This evolution is consistent with a high-porosity, layered target, which is also inferred from the high-resolution imaging of the impact point. Because of the low impact angle for DI (between 25° and 35° from the surface horizontal), changing styles of ejecta with time are mapped out spatially by the ballistic ejecta. Such changing styles provide qualitative but critical clues for scaling including initial coupling (plume evolution, shallow versus deep coupling) and excavation stages (symmetric versus asymmetric, non-radial rays). Two different approaches are used to constrain the final crater size: backward ray traces to the surface and estimates derived from the total ejected mass from earth-based telescopic observations. Ejecta ray traces indicate a diameter of about 175m. The total ejected mass based on Earth-based observations (107 kg dust and water ice) should be 50 times less than the total displaced mass for the crater (neglecting the contribution by ices). Based on this (and other considerations), the crater diameter could be a maximum of 250m. Nevertheless, the excavated mass observed from the earth (or other probes) most likely was derived from a very small fraction (and likely the upper surface) due to the oblique trajectory. The crater may very well be a nested crater, i.e., a deep penetration funnel surrounded by a shallow excavation crater.

11:00AM M4.00002 Impact Cratering Physics at Large Planetary Scales1. THOMAS J. AHERNS, Seismological Laboratory MS 252-21, California Institute of Technology, Pasadena, CA 91125 — Present understanding of the physics controlling formation of ~103 km diameter, multi-impacted ring structures on planets were derived from the ideas of Scipps oceanographer, W. Van Dorn, University of London’s, W. Murray, and, Caltech’s, D. O’Keefe who modeled the vertical oscillations (gravity and elasticity restoring forces) of shock-induced melt and damaged rock within the transient crater immediately after the downward propagating hemispheric shock has processed rock (both lining, and substantially below, the transient cavity crater). The resulting very large surface wave displacements produce the characteristic concentric, multi-ringed basins, as stored energy is radiated away and also dissipated upon inducing further cracking. Initial calculation description, of the above oscillation scenario, has focused upon on properly predicting the resulting density of cracks, and, their orientations. A new numerical version of the Ashby–Sammis crack damage model is coupled to an existing shock hydrodynamics code to predict impact induced damage distributions in a series of 15–70 cm rock targets from high speed impact experiments for a range of impactor type and velocity. These results are used to result of crack damage distributions induced in crustal rocks with small arms impactors and mapped ultrasonically in recent Caltech experiments (Ai and Ahrens, 2006).

11:30AM M4.00003 Shock compression of iron foils to Earth core conditions with GEKKO-HPER laser. KEISUKE SHIGEMORI, Institute of Laser Engineering, Osaka Univ., TETSUO IRIFUNE, Geodynamics Research Center, Ehime University, DAIGO ICHINOSE, KAZUTO OTANI, TATSUHIRO SAKAIYA, HIROSHI AZECHI, KUNIOKI MIMA, Institute of Laser Engineering, Osaka Univ., JUSTIN WARK, University of Oxford, BERNARD REMINGTON, Lawrence Livermore National Laboratory — We have been developing an experiment to create the Earth core condition (>300 GPa, ~6000 K) with intense laser. Experiments were done on GEKKO-HPER laser facility which has twelve beams from one direction for planar target experiments. We irradiated iron foils with a shaped pulse by stacking laser beams with certain time delay between the beams. Shock parameters (stress, shock velocity, shocked temperature) were measured by velocity interferometer for any reflector (VISAR) and optical spectral pyrometer. We also measured the sound velocity of the shocked iron foils with side-on x-ray backlighting technique. The measured sound velocity (> 300 GPa, ~5000K) shows solid sound velocity (~11 km/s) in good agreements with previous seismic data. We also started to measure the crystal conditions of the shocked iron with x-ray diffraction technique. Preliminary results were obtained at a pressure of >15 GPa.

11:45AM M4.00004 Ejection mechanisms for Martian meteorites. PAUL S. DE CARLI, Sri International/University College London, AHMED EL GORESY, Bayerisches Geoinstitut, University of Bayreuth, ZHIDONG XIE, THOMAS G. SHARP, Arizona State University — At least 34 meteorites have been identified by their characteristic isotopic signature as originating on Mars. The Martian origin of these meteorites is not in dispute. It is generally accepted that the meteorites were ejected from Mars as a result of asteroid or cometary impacts. However, there is no agreement on the detailed mechanism by which these meteorites were accelerated to the Martian escape velocity of 5 km/s. The simplest mechanism, that the meteorites were accelerated by a strong shock, implies a minimum shock pressure of about 65 GPa. Evidence from the meteorites themselves implies that none of them have been subjected to shock pressures in excess of about 40 GPa. Measurements of the magnetic properties of Martian meteorite ALH 84001 indicate that the ejection event did not heat it above its Curie temperature of about 40°C, implying a maximum shock pressure during ejection of less than 13 GPa. We have not been able to reproduce recent calculations that predict high velocity low pressure spalls. We explore the possibility that Martian meteorites are accelerated to escape velocity in a high velocity vapor or ejecta cloud.

12:00PM M4.00005 Improved Strength and Damage Modeling of Geologic Materials. SARAH STEWART, LAUREL SENFT, Department of Earth and Planetary Sciences, Harvard University — Collisions and impact cratering events are important processes in the evolution of planetary bodies. The time and length scales of planetary collisions, however, are inaccessible in the laboratory and require the use of shock physics codes. We present the results from a new rheological model for geological materials implemented in the CTH code [1]. The ‘ROCK’ model includes pressure, temperature, and damage effects on strength, as well as acoustic fluidization during impact crater collapse. We demonstrate that the model accurately reproduces final crater shapes, tensile cracking, and damaged zones from laboratory to planetary scales. The strength model requires basic material properties; hence, the input parameters may be benchmarked to laboratory results and extended to planetary collision events. We show the effects of varying material strength parameters, which are dependant on both scale and strain rate, and discuss choosing appropriate parameters for laboratory and planetary situations. The results are a significant improvement in models of continuum rock deformation during large scale impact events. [1] Senft, L. E., Stewart, S. T. Modeling Impact Cratering in Layered Surfaces, J. Geophys. Res., submitted.

12:15PM M4.00006 ABSTRACT WITHDRAWN

12:30PM M4.00007 Heterogeneous Thermal Emission from Shocked Basalt. SARAH STEWART, Harvard University, ACHIM SEIFTER, Los Alamos National Laboratory, GREGORY KENNEDY, Harvard University, MICHAEL FURLANETTO, ANDREW OBST, Los Alamos National Laboratory — Natural flaws in geologic materials result in heterogeneous pressure and temperature distributions upon shock compression. The effects of flaws are apparent in the thermal emission from shocked samples. We present emission temperature measurements from Columbia River Basalt using multi-band pyrometry (0.65 nm to 4.8 μm) and gated infrared imaging. After release from peak shock pressures between 9.5 and 45 GPa, free surface thermal emission temperatures range from 450 to >1250 K. The emission measurements show a departure from a quasi-single temperature surface between 10 and 14 GPa, where, at pressures well below that required for bulk melting of basalt, emission temperatures >1600 K are detected. In this pressure range, partial melting in fractures and pore spaces produce a bimodal temperature distribution comprised of a continuum and hot spots. The inferred hot spot distributions are in excellent agreement with petrographic studies of localized melting and generation of high pressure phases in basaltic meteorites from Mars shocked to similar pressures. However, the measured continuum temperatures in Columbia River Basalts are 100 to 400 K higher than inferred for Martian meteorites.
12:45PM M4.00008 Soft X-ray – Induced Shock Loading of Meteorite and Planetary Materials  
JOHN REMO, Depts. of Astronomy and E&S, Harvard University. MICHAEL FURNISH, Sandia National Laboratories — The response of meteorite and planetary materials to high intensity <1 keV x-rays from Z-pinch sources is described. These materials include iron and stony meteorites, magnesium rich olivine (dunite), and Al and Fe calibration samples. Input stresses varied from 6.1 to 12.4 GPa, attenuating to ~ 1.4 to 2.5 GPa for the iron meteorites, ~ 0.3 to 1.9 GPa for the stony meteorites, and 1.64 to 1.91 GPa for dunite. The calibration (pure) metals showed less attenuation than the highly inhomoogeneous natural materials. 9.5 to ~ 5 GPa for Fe and 12.4 to 10.6 GPa for Al. Putative equations of state are computed from Hugoniot pressure and shock velocity as a function of particle velocity. These data are useful for planetary and astrophysical modeling and for near-Earth object mitigation studies requiring momentum coupling, and momentum enhancement coefficients. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Wednesday, June 27, 2007 10:30AM - 12:15PM  
Session M5 Equation of State III Fairmont Orchid Hotel Plaza III

10:30AM M5.00001 Computational study of the equation of state of hydrogen using the Coupled Electron-Ion Monte Carlo Method  
MIGUEL MORALES, Department of Physics, University of Illinois at Urbana-Champaign, KRIS DELANEY, Materials Research Laboratory, UCSD, DAVID CEPERLEY, Department of Physics, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, Dipartimento di Fisica, Universita del l’Aquila, l’Aquila, Italy — We study the equation of state of liquid hydrogen at Mbar pressures, in the regime of pressure dissociation/ionization, using the Coupled Electron-Ion Monte Carlo (CEIMC) method. Our aim is to accurately describe the crossover from the molecular to the atomic regime. The CEIMC method is based on the Born-Oppenheimer approximation and consists of a Monte Carlo simulation of the ionic degrees of freedom (either with path integrals or classical Metropolis) using a potential energy surface obtained from a zero temperature QMC method. The electronic calculation is done using either Variational Monte Carlo or the more accurate Reptation Quantum Monte Carlo. A Slater-Jastrow wavefunction is used, with an analytical RPA Jastrow term and one-body orbitals, obtained from a fast band structure calculation, with backflow corrections. In addition to the thermodynamic and structural properties of the dense fluid, we will discuss the influence of quantum effects on the protons. We also compare our results with recent calculations obtained using Born-Oppenheimer Molecular Dynamics.

10:45AM M5.00002 The effect of functionals on the Equation of State using Density Functional Theory cold curves  
ANN E. MATTSSON, JOHN H. CARPENTER, Sandia National Labs, NM — With increasing computer power more complicated systems can be investigated by modeling and simulation efforts. These demanding simulations put unprecedented strain on the Equation of State (EOS). EOS models that have been perfectly adequate for smaller simulations can fail in unexpected ways for these more challenging applications. With the aim of improving the EOS, models are often fitted to calculated data in parts of the parameter space where little or no experimental data is available. For example, data calculated with the Quantum Molecular Dynamics (QMD) technique may be used in the warm dense matter regime. In this paper we focus on another type of calculated data, cold curves calculated with Density Functional Theory (DFT). The ultimate accuracy of a DFT or QMD calculation, although QMD is not addressed here, is governed by the choice of approximation for the exchange-correlation energy functional that embodies all many-body effects. We will discuss how the accuracy of the approximate functionals, manifested in the calculated cold curves, translate into accuracy for the EOS in different parts of the parameter space.

11:00AM M5.00003 Analysis of Cold Curve Forms for High–Pressure Physics  
JOHN CARPENTER, Sandia National Laboratories, IGOR LOMONOSOV, Institute of Problems of Chemical Physics RAS — An extensive collection of cold curve forms is analyzed using aluminum as a representative material. The cold pressure curves are compared with theoretical calculations up to 100 fold compressions. Furthermore, the effect of the curves on the Al Hugoniot at pressures of up to 100 Mbar is compared with a sampling of the available experimental data. An optimal cold curve form for equation of state applications is developed which describes the correct behavior near normal density and also in the asymptotic compression limit.

11:15AM M5.00004 Estimate of shock Hugoniot adiabat of liquids from hydrodynamics  
ERIC BOUTON, CEA, Le Ripault, BP 16, 37260 Monts, France, PIERRE VIDAL, Laboratoire de Combustion et detonique, UPR 9028 CNRS, 86960 Futuroscope, France — Predicting the Hugoniot shock states in liquids is of fundamental importance for numerical simulations and experimental investigations. Shock states are generally obtained from shock velocity (D) and material speed (u) measurements. In this paper, we propose two hydrodynamical methods for estimating the (D-u) Hugoniot curve of liquids from easily measured properties of the initial state. The first method is based upon the well-known experimental fact that for many liquids the shock adiabat is unique in a normalized plot. We then propose a quadratic form for this universal Hugoniot with only two parameters derived from physical considerations without fitting the experimental data. This relation is valid for liquids that do not undergo shock-induced phase under shock-pressure. The second method is based upon the differentiation of the Rankine-Hugoniot relations with the initial temperature considered as a variable and under the constraint of a unique nondimensional shock adiabat. We then obtain an ordinary differential equation (ODE) for the shock velocity D in the variable u. Upon integration, both methods predict the shock Hugoniot of liquid Nitromethane with a 10% accuracy for any initial temperature varying in the range from 250 K to 360K.

11:30AM M5.00005 A Finite Strain, Non-Reactive EOS for PBX9502  
BRIAN LAMBourn, NICHOLAS WHITWORTH, CAROLINE HANDLEY, HUGH JAMES, AWE plc — Like some liquids, the shock velocity - particle velocity relation for PBX9502 is initially curved, but tends to a linear relation for stronger shocks. Because of this, the method developed by Jeanloz of finding a Taylor expansion form for the principal isentrope cannot be used to develop an equation of state (EOS). Instead, the principal isentrope has been found from the Hugoniot by integration, using an analytic form for the variation of Gruneisen Gamma with specific volume. The isentrope has been extended by plausible extrapolations, both beyond the principal isentrope and the (D-u) Hugoniot curve of liquids from easily measured properties of the initial state. The first method is based upon the well-known experimental fact that for many liquids the shock adiabat is unique in a normalized plot. We then propose a quadratic form for this universal Hugoniot with only two parameters derived from physical considerations without fitting the experimental data. This relation is valid for liquids that do not undergo shock-induced phase under shock-pressure. The second method is based upon the differentiation of the Rankine-Hugoniot relations with the initial temperature considered as a variable and under the constraint of a unique nondimensional shock adiabat. We then obtain an ordinary differential equation (ODE) for the shock velocity D in the variable u. Upon integration, both methods predict the shock Hugoniot of liquid Nitromethane with a 10% accuracy for any initial temperature varying in the range from 250 K to 360K.

11:45AM M5.00006 Equations of State of Dual Functional Mixtures Of Structural Energetic Materials  
SATHYA HANAGUD, RUSISLAVA ZAHARIEVA, Georgia Tech, XIA LIU, University of Florida — Currently, the electronic structure and the equation of state of metals can be determined by the use of the density functional theory. However, the subject is still an active research field for disordered materials like alloys. This paper, however, is concerned with mixtures like aluminum, nickel and nickel oxide and not alloys. In general the mixture can be disordered and the ratio of the constituents can vary to accommodate the needed application and the associated structural design. In this paper, the hydrodynamically computed equations of state of mixtures are obtained from first principles calculations. Specifically mixtures of aluminum and nickel or nickel oxide, titanium and silicon, with binders and porosity, are considered. First, EOS of individual components is determined. Then, a super cell is constructed by the use of other disordered theories but noting the fact that we are considering mixtures and not alloys. Methods similar to the direct sampling method, quasi-random structures method and virtual crystal approximation are used to represent proper mixture architecture, with porosity. The results are then bridged to continuum through statistical mechanics techniques and compared with the results obtained from continuum mixture theories. To determine thermal effects, lattice thermal contributions and electron thermal contributions are included. The transition states are also discussed.
12:00PM M5.00007 Analytical Equations of State for use in Hydro-Codes. JOHN MAW, AWE — Hydro-code users often need to decide whether to use a tabular or analytical equation of state (EOS) in simulations. Many good, wide range, tabular forms have been generated, particularly for metals, often based on ab-initio electronic structure calculations. For other materials, including alloys and organics, tables either do not exist or are of limited accuracy. Analytical EOS forms can be generated quickly for novel materials where tabular forms are not available but are only as good as the experimental data used to generate them. However, they do have the advantage that they can be easily modified to assess the sensitivity of simulations to EOS uncertainties. A tabular form can only be modified by re-generating the EOS from scratch. This paper considers a number of analytical EOS forms, with particular emphasis on those that give realistic descriptions of low density and off-Hugoniot states far from the regimes where they have been validated. The issues of robustness, an essential requirement of EOS for hydro-code simulations are addressed. Temperatures are not explicitly calculated in EOS of the form P(V,E) but may be required for use in material strength models. Simple methods are discussed for calculating temperatures that are thermodynamically consistent with an analytical EOS.

Wednesday, June 27, 2007 10:30AM - 12:30PM — Session M6 Detonation Propagation/Mechanical Response Fairmont Orchid Hotel Promenade I/II

10:30AM M6.00001 The Energy Diameter Effect. PETER VITELLO, P. CLARK SOUERS, LLNL — The diameter (size) effect is the well-known increase of detonation velocity with increasing radius. We ask if a similar effect is seen with the detonation energy. To see this, it is necessary to perform the Cylinder test on small-radius samples of non-ideal explosives, which detonate with a low velocity. We fired nine ammonium nitrate/aluminum and AN/NM Cylinder shots with diameters of 12.7 to 50.8 mm using Fabry and heterodyne velocimetry for the wall velocities and pins for the detonation velocity. It is the use of the ultra-narrow 12.7 mm copper cylinders that give us points low enough to be sure that the effect exists. We find that the detonation energies at the three standard Cylinder relative volumes (2.2, 4.4, 7.2) vary roughly as the square of the detonation velocity. This is confirmed in numerical simulation calculations. A simple derivation of the relations of energy, detonation velocity, reaction zone length and detonation rate are given. We define a generalized inverse radius that can be applied to data for both explosive cylinders and outwardly-detonating spheres. The relation that detonation rate is proportional to the diameter effect slope can be used to derive the inverse radius equation. This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

10:45AM M6.00002 Ignition and Growth Modeling of Detonating TATB Cones and Arcs*. CRAIG TARVER, STEVEN CHIDESTER, Lawrence Livermore National Laboratory — Abstract. The Ignition and Growth reactive flow model for the detonating triaminotrinobenzene (TATB)-based explosives LX-17 and PBX 9502 is applied to recent experimental data on converging conical charges plus confined and unconfined arc charges. The conical charges are at first overridden by the converging flow and then fall to detonate as the radial rarefaction wave slows the reaction rate. Unconfined TATB arcs detonate more slowly than cylindrical charges on the inner surface and exhibit large phase velocities on the outer surface. Confinement reduces but does not eliminate these effects. The model calculations reproduce these features and agree well with experimental detonation velocity and arrival time data. *This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

11:00AM M6.00003 Analysis of Wave Curvature and Rate Stick Experiments for Monomodal Explosives with Different Crystal Quality and Particle Size Characteristics1. GERRIT SUTHERLAND, Naval Surface Warfare Center, Indian Head Division — Wood-Kirkwood theory and computer simulations of rate stick and wave curvature experiments of two sets of monomodal explosives are presented. One set [1] included two explosives composed of RDX or reduced sensitivity RDX representing a range of crystal quality. The second set [2] of explosives had mean particle sizes of 6, 134 and 428 µm. Wood-Kirkwood theory was used to calculate the reaction zone width from the wave curvature experiments. Two-term ignition and growth reactive model simulations for the first set of experiments were performed. Ignition and growth parameters were determined from embedded gauge experiments and critical diameter tests. The ability of the simulations to adequately predict shape of detonation velocity versus diameter curves and to replicate wave curvature data is presented. 1. G. T. Sutherland, 13th International Detonation Symposium, to be published. 2. H. Moulard, 9th International Detonation Symposium, pp. 18-24.

11:15AM M6.00004 Damage formation during high strain rate deformation of PBS9501. CLIVE SIVIOUR, University of Oxford, WILLIAM PROUD, University of Cambridge — A key aspect of the response of an explosive formulation to high strain rate loading is damage formation. In addition to the effect on immediate strength properties, damage, once formed, can lead to an undesirable increase in sensitivity and rate of burning. Methodologies for understanding and characterising the damage formed during loading are therefore vital if we are to claim a true understanding of the mechanical properties of these materials. This paper presents results from experiments on stimulant, PBS9501, of a polymer bonded explosive. High strain rate loading was performed in a split Hopkinson pressure bar, using speckle metrology and high speed photography to build up a more complete data-set on the formation of damage in this material. X-ray microtomography was also applied to examine internal damage in recovered specimens.

11:30AM M6.00005 The Dynamic Response of Energetic Formulations to Embedded Voids. GREGG GLENN, HORIE YASUYUKI, MICHAEL GUNGER, APS member — Programs are underway at AFRL and other labs to investigate the phenomenology of the response of energetic materials to long duration (>1 ms) loading environments. As part of these efforts, the effect of a defect, primarily in the form of a void, is the focus of the investigation. This paper will present a combined test and analytical study of multiple composite energetic formulations and will include a significant amount of test data. The primary variables associated with the loading environment are pressure, duration and loading rate. The energetic formulations primarily consist of ammonium perchlorate (AP), RDX, aluminum flake and HTPB binder. Void size and peak pressure were varied to determine safe loading margins. Post-test observations of reacted material were performed using a scanning electron microscope (SEM) to determine damage, crystal response and reaction locations within the sample. X-ray analysis was performed on unreacted samples to compare with reacted samples. The results are providing critical information on the sensitivity of an explosive formulation to void compression as a function of formulation, loading rate, peak pressure and duration. The results of these tests can be used in simulations to develop an improved understanding of mechanical and thermal initiation of energetic materials.

11:45AM M6.00006 Predicting Runaway Reaction in a Solid Explosive Containing a Single Crack. SCOTT JACKSON, LARRY HILL, Los Alamos National Laboratory — Mechanically damaged high explosive (HE) undergoing deflagration has been shown capable of generating combustion pressures and flame speeds dramatically in excess of those observed in undamaged HE. Flame penetration of HE cracks large enough to support the reaction zone increases the burning surface area and rate of gas production. Cracks confine the products, elevating the local pressure and reducing the reaction zone thickness such that it can enter continually smaller-width cracks. The process appreciably increases the flame surface area and rapidly pressurizes the crack network. This runaway of pressure and burning area, termed combustion bootstrapping, can dramatically accelerate the damage formation process and contribute to the onset of reaction runaway in a narrow HE slot intended to simulate a well-formed crack. We discuss experiments where flames were observed to propagate through such slots at velocities up to 10 km/s, reaching pressures in excess of 1 kbar. Pressurization of the slot due to gas-dynamic choking is then used to predict the onset of runaway reaction. This model agrees with experimental pressure measurements of observed reaction runaway in slots.
12:00PM M6.00007 Non-Shock Initiation of Plastic Bonded Explosive: Experimental and Theoretical methods I, KARMEN LAPPO — The goal of this research is to develop an empirical matrix that relates the level of damage created by an impulsive load on an explosive to the level of violence it produces — confined or unconfined. To develop this matrix, the first phase of the research will focus on relating the projectile velocity to a level of violence. The second phase will then relate the projectile velocity to a level of damage. This will then link the level of damage to the level of violence based on the projectile velocity. The third and final phase is to implement the data into a computational model and then validate its ability to simulate impact scenarios of explosives, explosive components, and explosive systems.

12:15PM M6.00008 Reaction Zone Structure of Steady-State Detonation Wave for Tetranitromethane1, ALEXANDER UTKIN, VALENTINA MOCHALOVA, VICTOR GARANIN, Institute of Problems of Chemical Physics RAS — The investigation of the reaction zone structure at steady-state detonation in liquid TNM by means of laser interferometer VISAR was conducted. The initial density and detonation velocity of TNM were 1.64 g/cm$^3$ and 6.4 km/s respectively. Laser beam reflected from Al foil with thickness 7-400 mkm placed between the charge and water window. Velocity profiles with Von Neumann spike were determined. The transition from the reaction zone to unloading wave is smooth and it doesn’t allow to define correctly the parameters of Chapman-Jouguet point. Approximate reaction time is 300 ns, and pressure in Von Neumann spike (26.4 GPa) exceeds the pressure in Chapman-Jouguet point (14.5 GPa) 1.8 times. Behind the shock jump a maximum gradient of particle velocity is observed which is equal to $10^7$ 1/s, it is a typical value for powerful HE. Although TNM has low parameters in Chapman-Jouguet point and a large duration of chemical reaction zone, the high initial decomposition rate provides the existence of steady-state detonation front in tetranitromethane.

1The work was supported by ISTC, Project #3394.

Wednesday, June 27, 2007 10:30AM - 12:30PM — Session M7 Inelastic Deformation-Mostly Strain Fairmont Orchid Hotel Promenade III

10:30AM M7.00001 High strain rate response of an elastomer, TONG JIAO, RODNEY CLIFTON, STEPHEN GRUNSCHEL, Brown University, BROWN UNIVERSITY TEAM — Pressure-shear plate impact experiments have been conducted to study the mechanical response of an elastomer (polyurea) at very high strain rates: $10^7 - 10^8$ s$^{-1}$. Thin samples are cast between two hard steel plates. Longitudinal waves reverberating through the sample are used to determine the slope of the isentrope at compressive stresses greater than, say, 500 MPa - the pressure at impact. Release wave experiments, combined with plane wave simulations, are used to extend the isentrope into the tensile regime. Because the healing resistance of polyurea depends strongly on pressure, two approaches are used to investigate the regime of high shear rate and low pressure. First, an unloading longitudinal wave reflected from the rear surface of the target assembly is made to arrive at the sample midway through its loading by the incident shear wave. As a result, the sample is sheared at high strain rates and both high and low pressure during a single experiment. Second, the thickness of the flyer and front plates are selected such that the compressive pulse passes through the cast-in-place sample before the shear wave arrives, allowing the shearing resistance to be measured at zero pressure. Results of these experiments and their simulation will be presented.

10:45AM M7.00002 Finite element based micromechanical modeling of brittle materials under compressive loading, REUBEN KRAFT, The Johns Hopkins University, JEAN-FRANCOIS MOLINARI, Ecole Normale Superieure de Cachan, K.T. RAMESH, The Johns Hopkins University — The performance of brittle materials is tightly linked to damage mechanisms at microstructural length scales. Thus, robust micro-level models are needed to adequately describe macro-level performance for materials many times subjected to extreme loading conditions. With a focus on brittle fracture under compressive loading, this presentation discusses the results of a numerical framework designed to model damage evolution at the microstructural level. A two-dimensional plane strain finite element model has been developed in which intergranular cracking is explicitly modeled using cohesive interfaces with well-characterized material parameters and an optimized contact algorithm. Effects of confinement, friction, strain rate, and spatial distribution of flaws on the macroscopic strength will be presented. In addition, the inhomogeneity of damage evolution is observed through use of the microstructure's dual graph providing valuable insight into the damage process.

11:00AM M7.00003 A Novel integrated experimental-numerical method for characterisation of materials at high strain rates, BEN ELLIOTT, ARIN JUMPASUT, NIK PETRINIC, CLIVE SIVIOUR, University of Oxford — Accurate prediction of material response at high strain rates necessarily requires an integrated approach to developing, calibrating and validating constitutive models. Experimental characterisation is a challenging task and simplified analyses inherently contain a number of unrealistic assumptions. These lead to results that are insufficiently accurate for use in challenging industrial design such as that found in aerospace applications. These problems can be avoided by the use of an integrated experimental-numerical approach which explicitly models non-ideal aspects of the characterisation procedures. This paper will demonstrate such an approach, where the problem is addressed by solving a related inverse problem. Calibration experiments and instrumentation thereon must be carefully chosen to provide appropriate information for a suitable numerical model of the material. In this case, Hopkinson bar experiments at various temperatures were used in conjunction with high speed photography and image processing to provide accurate experimental data. These were used directly within numerical models of the experiments in order to form a problem that could be accurately solved using inverse methods to yield useful physical material information. The properties obtained and material models chosen were validated using an experiment sufficiently complex to be industrially meaningful.

11:15AM M7.00004 Atomistic simulation of plasticity, spall damage and fracture of crystalline and polycrystalline metals under high strain rate1, GENRI NORMAN, Joint Institute for High Temperatures of RAS, Moscow, Russia — Modeling and simulation of dynamic atomic phenomena and processes in condensed matter are considered, which accompany intensive shock compression and release, uniaxial and hydrostatic stretching. Standards are presented for molecular dynamics (MD) modeling and simulation of relaxation processes: (1) the choice of system sizes, particle numbers and boundary conditions is discussed with respect to the spatial and temporal requirements and restrictions imposed by correlation lengths and correlation times of the processes to be modeled; (2) instantaneous and time averaged diagnostics are considered, spatial resolution included. The diagnostics includes study of (a) time evolutions of distributions of macroparameters (stress, temperature etc.) and structural characteristics (dilatation motion, void growth); (b) deviations of atom velocity and position distributions from the equilibrium ones etc. A hierarchy of dynamic and stochastic processes is introduced by the comparison of time scales with the dynamic memory time (predictability limit) which appears as a result of the Lyapunov instability of particle trajectories. Some theoretical MD based multi-scale approaches are presented which could be used to extend the MD results to the larger spatial and temporal scales. Examples are presented for Al, Fe, pure and Al doped Cu, and some other species for both perfect and defected crystals. The EAM potentials are mostly deployed. Comparisons with the experimental data available as well as with the simulation results of other authors are given.

1This work was partially supported by the RFBR grant 05-08-65423, RAS programs # 3, 9 and 14, and SNL under the US DOE/NNSA ASC program.
The dependence of the results on the average grain size, orientation and shape is studied.

A user facility is for everyone, national labs and universities. In fact, this is one way to facilitate involvement of people from national and military laboratories in basic research. The purpose of this town hall meeting is to solicit input from the community on what new things should be done in the applied research. A user facility can provide a process of crystal homogeneous melting and further cavitation in the melt formed. With the help of the models developed shock-wave loading is modeled and dynamic and static deformation processes are modeled: hydrostatic and uniaxial strain and shock wave loading in the impactor-target model. The dependence of the results on the average grain size, orientation and shape is studied.

This work was partially supported by the RFBR grant 05-08-65423, RAS programs #3, 9 and 14, and SNL under the US DOE/NNSA ASC program.

12:00PM M7.00006 Modeling of Al crystal fracture under high-rate strain based on atomistic simulations1, ALEXEY KUKSIN, GENRI NORMAN, VLADIMIR STEGAIOV, ALEXEY YANILKIN, Joint Institute for High Temperatures of RAS, Moscow, Russia — The recent experimental results [G.I. Kanel et al. // J. Phys.: Cond. Mat. 16 (2004) S1007] show the essential influence of the nanoprecipitates on spall strength of copper single crystals. In this work we address this issue by the molecular dynamics study. The models under consideration are the EAM systems of Al nanoclusters in the Cu matrix and Cu clusters in the Al matrix. We consider these two cases as the representative examples of nanocluster-matrix difference in shear strength. Three ways of the high strain rate deformation modeling are studied: hydrostatic and uniaxial strain and shock wave loading in the impactor-target model. The preexisting edge dislocation interaction with the precipitate under shear deformation is addressed. The effect of the precipitate size is considered.

This work was partially supported by the RFBR grant 05-08-65423, RAS programs #3, 9 and 14, and SNL under the US DOE/NNSA ASC program.

12:15PM M7.00007 Atomic study of nanoprecipitates influence on plasticity and fracture of crystalline metals1, VLADIMIR STEGAIOV, ALEXEY KUKSIN, GENRI NORMAN, ALEXEY YANILKIN, Joint Institute for High Temperatures of RAS, Moscow, Russia — The recent experimental results [G.I. Kanel et al., 2006] show the essential influence of the nanoprecipitates on spall strength of copper single crystals. In this work we address this issue by the molecular dynamics study. The models under consideration are the EAM systems of Al nanoclusters in the Cu matrix and Cu clusters in the Al matrix. We consider these two cases as the representative examples of nanocluster-matrix difference in shear strength. Three ways of the high strain rate deformation modeling are studied: hydrostatic and uniaxial strain and shock wave loading in the impactor-target model. The preexisting edge dislocation interaction with the precipitate under shear deformation is addressed. The effect of the precipitate size is considered.

This work was partially supported by the RFBR grant 05-08-65423, RAS programs #3, 9 and 14, and SNL under the US DOE/NNSA ASC program.

Thursday, June 28, 2007 8:00AM - 8:30AM  
Session N1 Shock Science Award  
Fairmont Orchid Hotel Salon 1/II

8:00AM N1.00001 The Shock Wave Profile: Causes and Effects, DENNIS GRADY, Applied Research Associates — Causes of the shock wave profile are well known. So are many of the effects. If there were a symbol and a logo pertaining to shock compression science, it would probably be the shock wave profile. In condensed matter, the shock wave profile assumes many shapes and forms. Metal, rock, ceramic, plastic, and energetic materials all impose their unique properties onto the structure of the shock wave profile. Experimental visualization of the shock wave profile has proved a daunting task. So has interpretation of the underlying physics. Every rise, fall, hesitation and inflection of the shock wave profile has meaning. Some of these features are beginning to understand. The presentation is centered about the author's efforts to extract physics from the shock wave profile over the past four decades.

Thursday, June 28, 2007 9:00AM - 10:00AM  
Session P1 Town Hall Meeting on Future Directions in Dynamic High Pressure Research  
Fairmont Orchid Hotel Salon 1/II

9:00AM P1.00001 Town Hall Meeting on Future Directions in Dynamic High Pressure Research, W.J. NELLIS, Harvard University — Dynamic compression research began in the U. S. sixty years ago. The motivator was national defense and compression was accomplished by a single shock wave. Since that time the world has changed substantially. New issues, in addition to military ones, threaten international stability in the twenty-first century. Isentropic and quasi-isentropic compression techniques have now been developed, which means temperature can be tuned independent of pressure between that on the Hugoniot and that on the isentrop. States can be achieved by dynamic compression that cannot be achieved by other methods. Dynamic and static compression with laser heating can now be used to measure different properties at the same conditions. The time is right for a national user facility in an unclassified University environment that achieves extreme conditions of high-energy density in condensed matter. Such facilities currently exist mainly in National Laboratories and should be developed in an open, unclassified University environment for fundamental and applied research. A user facility is for every one, national labs and universities. In fact, this is one way to facilitate involvement of people from national and military laboratories in basic research. The purpose of this town hall meeting is to solicit input from the community on what new things should be done in the future with dynamic compression. Anyone who would like to present a suggestion will have about five minutes to do so, depending on the number of people wishing time and the time available.

Thursday, June 28, 2007 10:30AM - 12:00PM  
Session P2 Material Science III  
Fairmont Orchid Hotel Amphitheater
10:30AM P2.00001 Microstructural Evolution and Phase Stability in Shock-Loaded Tantalum Single Crystals, JIKOU ZHOU, CHENG SAW, RICKY CHAU, LUKE HSUNG, Lawrence Livermore National Laboratory — Deformation of tantalum and tantalum alloys has been studied repeatedly in order to understand their constitutive behavior and microstructural stability under dynamic pressure conditions. Shock-induced microstructures including dislocation patterning, deformation twinning, and phase change have been reported in shock-deformed poly-crystalline tantalum, and the strain hardening of post-shocked polycrystalline tantalum was mainly attributed to deformation twinning. However, the underlying mechanisms for shock-induced deformation twinning remain unclear. In this presentation, we report the results of a systematic study, which investigate the microstructural evolution and mechanical properties of shocked tantalum single crystals. Shock impact experiments were carried out in a two-stage gas gun under three different pressures: 25 GPa, 50 GPa and 70 GPa. The effects of crystal orientation and pressure on deformation substructures and mechanical properties are investigated by analyzing shock-recovered samples using x-ray diffraction, nanoindentation, and transmission electron microscopy techniques. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

10:45AM P2.00002 Fabrication of W-Cu/Mo-Cu functionally graded materials by explosive consolidation, PENGWAN CHEN, ZHIMING JIANG, Beijing Institute of Technology, WEIPING SHEN, Beijing University of Science and Technology, JUN YANG, FENGLEI HUANG, Beijing Institute of Technology — Attempts are made to use explosive consolidation to fabricate high quality W-Cu/Mo-Cu FGMs. Tungsten powder with 99% purity and a particle size of 3~25µm and molybdenum/copper powder with >99% purity and a particle size of 74µm are used as starting powder. A novel technique, called bidirectional underwater shockwave explosive consolidation, is developed. Two water chambers are placed in both sides of the sample. Detonation-generated shock waves are attenuated by the water chambers before acting on the samples. Through adjusting the height of the water columns, the applied pressure can be adjusted. A self-propagating reaction system is used to provide temperature compensation and to enhance consolidation quality. Flash X-ray photography is used to observe the process of explosive consolidation. Various techniques are used to characterize the recovered samples including optical microscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD), energy spectrum analysis, hardness measurement and density measurement. The explosive consolidation methods developed in the paper can be used to other hard-to-consolidate powder materials.

11:00AM P2.00003 Comparison of Porter-Gould constitutive model with Compression Test data for HTPB/Sugar, PHILIP CHURCH, PETER GOULD, WILLIAM HUNTINGTON-THRESHER, QinetiQ, DANIEL DRIDGE, WILLIAM PROUD, University of Cambridge — QinetiQ has been developing the physically based QinetiQ Porter-Gould (P-G) model for the mechanical response of PBXs over a number of years and applying to solving real scenarios involving impact and blast. The main difficulty with these models is predicting the intermediate strain rate regime where the relaxation time for the polymer is of the same order as the duration of the Hopkinson bar test. The other main issue is the ability of the model to predict the loss of energy data as a function of temperature up to and through the glass transition temperature. The paper presents predictions from the QinetiQ P-G model compared to quasi-static compression and Hopkinson bar compression test data and discusses the results in terms of requirements for future developments of the model.

11:15AM P2.00004 Microstructural Defects in Shocked Nanocrystalline Ni and Ni-W, HUSSAM JARMAKANI, UCSD, EDUARDO BRINGA, MORRIS WANG, LLNL, CHRIS SCHUH, MIT, MARC MEYERS, UCSD — This mechanisms of defect generation and multiplication in nanocrystalline Ni and Ni-W deformed at very high strain rates between \( \varepsilon \sim 10^4 \text{sec}^{-1} \) and \( \varepsilon \sim 10^7 \text{sec}^{-1} \) quasi-isentropically compression via gas-gun and laser methods are investigated experimentally, experimentally, and computationally. Transmission Electron Microscopy (TEM) was used to probe the recovered microstructure for defects (dislocations, stacking faults, twins, etc.). As the grain size is decreased and stacking-fault energy is increased, the propensity for twinning is decreased and the critical twinning pressure is increased. An analytical model was developed that determines the critical twinning pressure as a function of grain size and stacking-fault energy. Molecular dynamics (MD) simulations using LAMMPS were performed on nc Ni, and results of the defect structure are compared with that of TEM. This research effort is funded by grant no. LLNL-B560780.

11:30AM P2.00005 Influence of polyethylene molecular conformation on Taylor impact measurements: a comparison of HDPE, UHMWPE, and PEX, CARL P. TRUJILLO, ERIC N. BROWN, GEORGE T. GRAY III, Los Alamos National Laboratory, Materials Science and Technology Division, LOS ALAMOS NATIONAL LABORATORY, MATERIALS SCIENCE AND TECHNOLOGY DIVISION TEAM — The current work presents the comparison of the Taylor impact response of three different industrial forms of polyethylene. Specifically, high-density polyethylene (HDPE), ultra high molecular weight polyethylene (UHMWPE), and cross-linked polyethylene (PEX) were tested. From quasi-static and intermediate strain-rate compression measurements as a function of temperature (75 to 100°C) and strain-rate (10^-4 to 2600 s^-1) the responses of UHMWPE and PEX are very similar, whereas HDPE exhibits some differences. The HDPE samples display a significantly higher yield stress followed by a flat flow behavior. Conversely, UHMWPE and PEX both exhibit significant strain hardening after yield. Taylor impact experiments are presented as a function of velocity and temperature to probe the dynamic yield behavior and ductile-to-brittle response of these polymers.

11:45AM P2.00006 Propagation of strongly nonlinear signals in a two dimensional network of granular chains, CHIARA DARIAO, Aeronautics and Applied Physics, California Institute of Technology, VITALI F. NESTERENKO, Mechanical and Aerospace Engineering Department, University of California, San Diego — We report experimental observation of strongly nonlinear signals propagating in a two dimensional system composed of guided granular chains. In this system one of the chains contacts two others to allow splitting and redirecting the solitary-like signal formed by impact on the first chain. The system consists of a double Y-shaped guide in which high- and low-modulus chains of spheres are arranged in various geometries. We observed fast splitting of the initial pulse, rapid chaotization of the signal and sharp bending of the propagating acoustic information. Pulse and energy trapping in the branches was also observed in composite systems assembled from hard- and soft-particles.

Thursday, June 28, 2007 10:30AM - 12:15PM
Session P3 Phase Transitions III Fairmont Orchid Hotel Plaza I

10:30AM P3.00001 Electronic Conduction of Tin Under High Pressure from A phenomenological-Equation of State, SHLOMI PISTINNER, Prop. Div. Soreq NRS Yavne Israel — Phase transition under shock loading, and unloading are indirectly inferred from a abrupt change in the speed of sound. To estimate this change we use the Tin thermodynamic-phenomenological equation of state, obtained by Mabire and Heril (SCCM 2000). Mabire and Heril have demonstrated the ability of this equation of state to reproduce VISAR profiles obtained in impact experiments. The parameters of this equation of state are worked out in the frame work of Debye theory and converted to parameters usable in the Bloch-Grueisen DC resistivity formula. This quantity is then used in Drude AC resistivity model to infer a wavelength dependent emissivity. The emissivity so inferred can be used to reduce uncertainties in temperature which is inferred from pirometric measurements at shocked Tin unloading. This can be done in a manner consistent with the process of state. In print the prediction of the exercise carried out below are verifiable via independent measurements of an angle dependent emissivity via techniques such as ellipsometry.
10:45AM P3.00002 Free Surface Temperature Measurements on Shock loaded Tin (Melting on Release) , ACHIM SEIFTER, ANDREW OBST, DAVID HOLTKAMP, Los Alamos National Laboratory, DALE TURLEY, Special Technology Laboratory, Santa Barbara, MIKE FURLANETTO, JEREMY PAYTON, CARL GREEFF, Los Alamos National Laboratory — Theory predicts that over a certain range of Hugoniot pressures the free surface temperature of shock loaded tin is the ambient pressure melting temperature of 505K. In a series of high explosive driven (direct drive) shocks into tin of various thicknesses we attempted to measure this constant temperature. From the lower end (195kbar) up to the middle (250kbar) of this pressure range we could observe this temperature within the uncertainty of our measurements. From about 250kbar up to the higher end (330kbar) the measured free surface temperature was increasing with increasing Hugoniot pressure. In this paper we will describe the experimental setup, the diagnostic systems (pyrometry and Photon Doppler Velocimetry) and give possible explanations for the temperature readings higher than the predicted 505K in the upper half of the investigated pressure range.

11:00AM P3.00003 Measurements of the Dynamic $\beta \rightarrow \gamma$ Phase Boundary in Tin$^1$ , JEAN-PAUL DAVIS, DENNIS B. HAYES, Sandia National Laboratories, Albuquerque NM 87185 — Experiments performed on the Z machine at Sandia Labs used magnetically generated planar ramp waves to quasi-isentropically compress pre-heated solid tin across the equilibrium $\beta \rightarrow \gamma$ phase boundary. Velocity history measurements at a tin/window interface exhibited features that could be consistently related, through simulations, to the $\beta \rightarrow \gamma$ structural transformation occurring in the bulk tin. The simulations used a homogeneous phase-mixture model with a $\gamma$-phase energy offset that was adjusted to match the measured velocity feature. This determined the phase-boundary pressure from experiment and the phase-boundary temperature from the $\beta$-phase equation of state. Due to wave interactions, measurements using sapphire windows were more difficult to interpret than those using LiF windows and thus led to results with larger uncertainty. The measured phase boundary pressure did not depend on the tin’s initial microstructure, nor on perturbations to the wave profile arising from the difficulty of pre-heating a soft metal in the isentropic compression configuration.

1$^1$Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:15AM P3.00004 Atomistic Simulations of Shock Waves in Polycrystalline Iron Compared to Experiments$^1$ , KAI KADAU, T.C. GERMANN, P.S. LOMDAHL, R.C. ALBERS, LANL, J.S. WARK, A. HIGGINBOTHAM, University of Oxford, B.L. HOLIAN, LANL — The propagation of shock waves through a polycrystalline iron sample is explored by large-scale atomistic simulations. For large enough shock strengths the passage of the wave causes the body-centered-cubic (bcc) structure to transform into a close-packed structure with most structure being isotropic hexagonal-close-packed (hcp) and, depending on shock strength and grain orientation, some fraction of face-centered-cubic (fcc) structure. The simulated shock state as represented by the Hugoniot is compared to experimental data. By calculating the extended x-ray absorption fine structure (EXAFS) directly from the atomic configurations obtained by our simulations, a comparison to recent experimental EXAFS measurements of nanosecond-laser shocks in polycrystalline iron shows that the experimental data is consistent with a phase transformation. However, the atomistically simulated EXAFS spectra also show that an experimental distinction between a product hcp or fcc phase is not possible based on the EXAFS spectra alone.

$^1$This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

11:30AM P3.00005 Recovery Studies of Shocked Iron Single Crystals$^1$ , BASSEM EL-DASHER, NATHAN BARTON, WARREN MOBERLYCHAN, JAMES MCNANEY, JAMES HAWRELIAK, HECTOR LORENZANA, Lawrence Livermore National Laboratory — Time resolved, in-situ X-Ray diffraction measurements indicate that the bcc-hcp transition in single crystal iron occurs at about 13 GPa. These results also show that the high pressure phase is a polycrystal with two variants. Further studies on the recovered specimens using transmission electron microscopy show that these shocked samples surprisingly reverse transform from a high pressure polycrystal to the original single crystal structure upon release. These results will be discussed in the context of the time resolved data and theoretically based transformation pathways.

$^1$This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48. The project (06-SI-004) was funded by the LDRD Program at LLNL.

11:45AM P3.00006 ABSTRACT WITHDRAWN —

12:00PM P3.00007 Effect of nano-void on the phase transformation of single crystal iron under shock compression$^1$ , XINLIN CUI, WENJUN ZHU, HONGLIANG HE, YINGJUN LI — Shock-induced phase transformation (body-centered cubic $\alpha$ phase to hexagonal close-packed $\varepsilon$ phase) in single crystal iron has been investigated by means of the molecular dynamics (MD) simulation using an embedded atom method (EAM) potential. By introducing a nano-void in the single crystal iron, the nucleation velocity and the nucleation sites are observed to be different from the ideal single crystal iron. The simulation results show that the void accelerates the nucleation velocity, which induces the new phase to nucleate easier. At the same time, the void affects the nucleation sites, the initial homogeneous nucleation is observed near to the leading front of the shock wave in the ideal single crystal iron, but they firstly occur around the edge of the void, and finally form a butterfly shaped transformation zone in the defect single crystal iron. By calculating the distribution of the resolved shear stress along the slip plane, the reason why the nucleation sites are different has been explained.

$^1$Project supported by the National Natural Science Foundation NSAF (Grant. No. 10476027) and by the Science and Technology Foundation of China Academy of Engineering Physics (Grant. No.20050105)

Thursday, June 28, 2007 10:30AM - 12:30PM –
Session P4 Inelastic Deformation IV Fairmont Orchid Hotel Plaza II

10:30AM P4.00001 Dynamic Plastic Response of Aluminum at Temperatures Approaching Melt , STEPHEN GRUNSCHEL, RODNEY CLIFTON, Brown University — This study uses the pressure-shear plate impact configuration to investigate the rate-controlling mechanisms of the plastic response of metals at strain rates on the order of $10^6$ s$^{-1}$ and at temperatures that approach melt. In similar experiments by Frutschy and Clifton (JOMPS 46, 1998, 1723-1743) on OFHC copper, the flow stress decreases with increasing temperature and increases with increasing strain rate over the full range of temperatures and strain rates examined. No conclusive evidence of a change in rate-controlling mechanism was obtained. In the current study, temperatures that are larger fractions of the melting temperature are accessible because of the lower melting point of aluminum. So far, the shear strain rate has been measured at temperatures up to 630 C, which is 81% of the melting temperature at the concurrent pressure. Several approaches are being explored to obtain even higher fractions of the melting temperature, possibly exceeding it. Results of these approaches will be presented.
1:00AM P4.00003 Transition from solid to liquid spall in tin under laser shocks of increasing intensity. THIBAULT DE RESSEGUIER, CNRS, LOIC SIGNOR, CEA Valduc, THIBAULT DE RESSEGUIER, LCD, ENSMA Poitiers, France, ANDRE DRAGON, PIERRE SEVERIN, MICHEL BOUSTIE, CNRS, LCD TEAM, CEA TEAM, LMPM TEAM — When a shock-loaded target is melted on compression or on release, the tensile stresses generated upon reflection of the pressure pulse from a free surface are induced in a liquid state. Instead of the well-known spallation process occurring in solid targets, cavitation takes place in the melted dynamic behavior of mortar. Longitudinal and lateral stresses have been directly measured by means of embedded polyvinylidene fluoride (PVDF) gauges up to 1 GPa. A 200 mm-cal. powder gun enable us to measure longitudinal and lateral stresses at several point from the impact surface, simultaneously. The shear strength under impact-loading has been obtained from measured longitudinal and lateral stresses. The longitudinal stress profile shows a two-wave structure. Experimental data are compared to theoretical predictions from hydrocode simulations coupled with a modified formulation of the well-known energy fragmentation model of D.E. Grady [J. Mech. Phys. Sol., 36(3), pp.353-384, 1988].

11:15AM P4.00004 Fragment-size prediction during dynamic fragmentation of melted tin. Experimental investigation and modelling issues. GILLES ROY, LOIC SIGNOR, CEA Valduc, THIBAULT DE RESSEGUIER, LCD, ENSMA Poitiers, France, ANDRE DRAGON, PIERRE SEVERIN, MICHEL BOUSTIE, CNRS, LCD TEAM, CEA TEAM, LMPM TEAM — In a recent paper, we have reported an exploratory investigation of liquid spall in tin samples submitted to laser shocks of very high intensities [J. Appl. Phys. 101, 013506, 2007]. Here, we present new experimental results obtained over a lower pressure range (~14 to 60 GPa), where we focus on the progressive transition from the ductile behaviour of solid tin to the cavitating spall expected above melting. Both time-resolved free surface velocity measurements and post-test examination of the recovered samples clearly show such transition. The drop in tensile strength associated with melting is evaluated from the velocity profiles. Detailed views of the fracture surfaces provide an insight into the cavitation process. Experimental data are compared to preliminary computations.

11:30AM P4.00005 The dynamic behavior of mortar under impact-loading. NOBUAKI KAWAI, KENJI INOUE, SATOSHI MISAWA, KYOJI TANAKA, SHIZUO HAYASHI, KEN-ICHI KONDO, Materials and Structures Laboratory, Tokyo Institute of Technology, WERNER RIEDEL, Fraunhofer, Ernst-Mach-Institut — Concrete and mortar are the most fundamental structural material. Therefore, considerable interest in characterizing the dynamic behavior of these materials is expected in the context of impact-loading exists. In this study, plate impact experiments have been performed to determine the dynamic behavior of mortar. Longitudinal and lateral stresses have been directly measured by means of embedded polyvinylidene fluoride (PVDF) gauges up to 1 GPa. A 200 mm-cal. powder gun enable us to measure longitudinal and lateral stresses at several point from the impact surface, simultaneously. The shear strength under impact-loading has been obtained from measured longitudinal and lateral stresses. The longitudinal stress profile shows a two-wave structure. It is indicated that this structure is associated with the onset of pore compaction and failure of mortar by comparing with hydrocode simulations using an elastic-plastic damage model for concrete.

11:45AM P4.00006 Phase Transition Behavior and Abnormal Spall in FeMnNi alloy with Low α − ε Transition Stress. HAIBO HU, YONGTAO CHEN, QINGZHONG LI, Institute of Fluid Physics, CAEP — Phase transition behavior of a FeMnNi alloy with low α − ε phase transition stress in range of 6~7GPa and corresponding spall phenomena are studied. Two experiment set up of symmetric impact design with flyer and target of same thickness and reverse impact technique of metal flyer on sapphire window are used. Loading and release wave profile are recorded with help of VISAR with two constants of strip numbers. Experiments are conducted on 100-mm-diameter and two stage light gas gun in velocity range from 300m/s up to 2000m/s. Discussion is focused on the formation of rarefaction shock wave and corresponding spall phenomena. It is shown that spallation may happen in symmetric impacts when stress is higher than phase transition point. In velocity range up to 2000m/s, when impacting stress is more than 40GPa and shock front is overdriven, a spallation like oscillation profile is noticed in domain of first plateau in velocity curve. As release wave from impact side should come some time later, it may be raised by reflection of release wave from free surface with reverse phase transition. Specimen is thoroughly broken, although pulse X-ray records at the moment of 14 μs after impact show no sign of multi-spallation. Further experiments are planned using VISAR with two constants of strip numbers to verify this phenomenon and parameters such as spall strength, spall thickness.

12:00PM P4.00007 Shock-induced turbulence and dissipative structures in copper1. YURI MESHCHERYAKOV, NATALI ZHIGACHEVA, ALEXANDRE DIVAKOV, INAN MAKAREVICH, Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, BORIS BARAKHTIN, Central Research Institute of Constructional Materials “Promety” — A shock-wave loading under uniaxial strain conditions of polycrystalline M3 copper reveals a threshold nucleation of dissipative structures of 15±25 μm in diameter. Where observed the turbulent-like formations lie in the grains favorable oriented respectively shock wave propagation direction. Each structure consists of networks of parallel or mutual perpendicular shear bands of 100−300 nm spacing, so the size of elementary cell restricted by shear bands in their scale belong to nanostructure. Macroscopically, momentum and energy expended on formation of the structures is quantitatively characterized by “deficit of particle velocity” - difference between impact velocity under symmetrical collision and free surface velocity of shock loaded plane target. There is a threshold strain rate higher which the deficit of particle velocity begins to grow very fast and simultaneously the hardness and spall-strength of material grow in the same manner.

1 Russian Foundation for Basic Researches.
12:15PM P4.00008 Influence of nano-size inclusions on spall fracture of copper single crystals. SERGEY RAZORENOV, Institute of Problems of Chemical Physics RAS, GENNADY KANEL, Joint Institute for High Temperatures, GALINA IVANCHIKHINA, Institute of Problems of Chemical Physics RAS, INSTITUTE OF PROBLEMS OF CHEMICAL PHYSICS RAS TEAM, JOINT INSTITUTE FOR HIGH TEMPERATURES TEAM — Spall experiments have been carried out for copper in different structural states. The samples were copper single crystals, crystals of Cu + 0.1% Si, copper crystals with silica particles of 180 nm average size, and polycrystalline copper. Shock pulses of 10−7 s to 10−7 s duration were generated by aluminum flyer plates 0.1 mm to 0.8 mm in thickness at 0.6 km/s to 1.2 km/s impact velocity. In experiments, the free surface velocity histories were recorded with the VISAR. Solid solution Cu + 0.1% Si demonstrates more prolonged spall process than pure copper crystals. At longer pulse durations its spall strength is slightly less than that of pure crystals but approaches the latter with decreasing pulse duration. Fracture of copper with silica inclusions is completed much faster. The spall strength of this material is close to that of Cu + 0.1% Si crystals and approaches the strength of polycrystalline copper with decreasing the load duration. Mechanisms and kinetics of the spall fracture process are discussed in the light of these new data. The work was supported by Russian Foundation for Basic Research, grant number 06-02-17057-a.

Thursday, June 28, 2007 10:30AM - 12:30PM — Session P5 Equation of State IV Fairmont Orchid Hotel Plaza III

10:30AM P5.00001 Systematics of Compression of Hard Materials1, W. J. NELLIS, T. PETACH, Harvard University — Hard materials are those for which the the Rayleigh line is close to Hugoniot, which means thermal pressures are small, which means Hugoniot, isentrope, and isotherm of a given material are nearly coincident up to 100 GPa pressures. Hard materials are used, for example, as anvils in reverberating shock experiments to look at quasi-isentropically compressed, highly-condensed low-Z fluids. For this reason, the shock impedances, optical transparencies, and electrical conductivities of these materials are of interest above 50 GPa. In this paper measured Hugoniot and isotherms of materials such as diamond, sapphire, titanium dioxide, GGG, etc will be used to derive systematic equation-of-state behavior for these materials. Major conclusions and future experiments will be discussed.

1This work was supported by the US Army Research Office

10:45AM P5.00002 Equation of State for Ti-Beta-21S, KEVIN HONNELL, NENAD VELISAVLJEVIC, CHRIS ADAMS, PAULO RIGG, GARY CHESNUT, ROBERT AIKIN, JR., JONATHAN BOETTGER, Los Alamos National Laboratory — A new, tabular, SESAME equation of state is presented for Ti-Beta-21S (TIMETAL 21S®), a high-strength, high-temperature, beta-stabilized alloy of Ti, Mo, Nb, and Al. The new equation of state combines an empirical, Vinet description of the cold curve with the Johnson ionic model and the Thomas-Fermi-Dirac model for the thermal electronic contributions. Both the HCP and BCC phases are accounted for via the cold curve. Predictions for the room-temperature isotherm, principal Hugoniot, and thermal expansion are compared to new experimental results.

11:00AM P5.00003 An Equation of State study of a Boron Nitride rubber composite using a Single Stage Gas Gun, PETER TAYLOR, PETER KEIGHTLEY, AWE Aldermaston, HYDRODYNAMICS DEPARTMENT TEAM — The equation of state of a Boron Nitride powder / Neoprene / Polythene composite has been determined experimentally up to 5GPa using a single stage Helium gas gun. The newly commissioned gun operates using a fast acting gas valve breech, and is capable of launching a 65mm diameter flyer at up to 1km/s. A series of 1D plate impact experiments has been employed using a shock reverberation or ring-up technique in which the sample is sandwiched between layers of a higher shock impedance material. Manganin stress gauges are used to measure the stress levels and shock arrival times as the shocks reverberate within the sample layer. The Hugoniot has been determined from the measured stress and shock velocity at several impact velocities for the first shock. Subsequent reflected shocks within the sample have been measured and used to determine off Hugoniot states and hence Gruniesen Gamma in order to derive the equation of state.

11:15AM P5.00004 On the applicability of analytical models to predict Hugoniot of nano-sized powder compacts,1, CHENGDA DAI, DANIEL EAKINS, NAresh THADHANI, Georgia Tech, HSRLAB TEAM — Hugoniot of nano-sized powder pre-pressed to varied porosities is crucial for design of shock compaction experiments to fabricate bulk consolidated nanostructured compacts and for validation of the equation of state over a wide range of density and temperature. The McQueen and Wu-Ling models are representatives of isochoric and isobaric approaches to predicting porous Hugoniot. Both models, however, neglect the difference in internal energy between the powder compact and solid. Hence, it is uncertain if the models can still be applied to predict the Hugoniot of nanoparticle compact due to the high specific surface energy of nanoparticles relevant to specific internal energy. In the present work, we review the two models, focusing on their main assumptions and resultant restrictions, and show the increasing deviation if the models can still be applied to predict the Hugoniot of nanoparticle compact due to the high specific surface energy of nanoparticles relevant to specific internal energy. In the present work, we review the two models, focusing on their main assumptions and resultant restrictions, and show the increasing deviation if the models can still be applied to predict the Hugoniot of nanoparticle compact due to the high specific surface energy of nanoparticles relevant to specific internal energy.

1This work was granted by ONR/MURI under No. N00014-05-1-0497.

11:30AM P5.00005 Shock compression and equation of state of C_{60} fullerite, VLADIMIR MLYAVSKY, KONSTANTIN KHISHCHENKO, IHED of IJHT RAS, ALEXANDER UTINKIN, VLADISLAV YAKUSHEV, IPCP RAS, ANDREY ZHUK, VLADIMIR FORTOV, IJHT RAS — Recently, we have experimentally studied shock compressibility of C_{60} fullerite and sound velocity in shock-compressed fullerite [1]. The Hugoniot of C_{60} fullerite had a set of peculiarities. Appearance of a rather hard carbon phase was detected at shock pressure ∼ 9 GPa. We assume that it is a 2D-polymerized C_{60} phase. With increase of shock pressure, destruction of this phase and formation of a graphite-like carbon occurs. With further increase of shock pressure, the graphite- like carbon transforms to a diamond-like phase. If shock pressure is higher than ∼ 33 GPa, shock compressibility of C_{60} fullerite is determined by the thermodynamic properties of the diamond-like phase. The results of the shock-wave measurements were used for the description of thermodynamic properties of C_{60} fullerite and products of its transformations in a wide range of pressures and temperatures. A semiempirical equation of state for the simple cubic phase of C_{60} fullerite is proposed. The EOS we have developed for fullerite C_{60} provides a consistent representation of the available experimental data. The work was supported by RFBR. [1] Mlyavsky V.V., Utkin A.V., Zhuk A.Z., Yakushev V.V. and Fortov V.E. Diamond and Rel. Mat. 14 (2005) 1920.

11:45AM P5.00006 Dynamic Loading of Teflon at 200°C, PAUL A. URTIEW, JERRY W. FORBES, CRAIG M. TARVER, KEVIN S. VANDERSALL, FRANK GARCIA, LAWRENCE LIVERMORE NATIONAL LABORATORY COLLABORATION, NAVAL SURFACE WEAPONS CENTER, INDIAN HEAD, MD AND UNIVERSITY OF MARYLAND COLLABORATION — Dynamic loading experiments were performed on inert Teflon (Polytetrafluoroethylene) samples, initially heated to the temperature of 200°C, to test its behavior under these conditions for their use in other heated experiments. Tests were performed in the 100 mm diameter bore propellant driven gas gun with piezo-resistive manganin pressure gauges imbedded into the samples to measure loading pressures. Experimental data provided new information on the shock velocity – particle velocity relationship for the heated material and showed no effect of temperature on the non-conducting property of the material being used as an electrical insulator. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.
12:00PM P5.00007 Shock Hugoniot Behavior for Particle Reinforced Polymer Composites, LOUIS FERRANTI, JR., NARESH THADHANI, Georgia Institute of Technology, JENNIFER JORDAN, RICHARD DICK, Air Force Research Laboratory (AFRL/MMNE) — The shock Hugoniot for polymers exhibits a non-linear \( U_S - U_P \) relationship at relatively low pressures, showing a concave curvature with an initially rapid shock velocity. In contrast, the shock Hugoniot for a particle reinforced polymer composite displays a convex curvature with initially rapid particle velocity. Transformation to pressure-volume space shows an initial expansion that is not related to a low-pressure phase change or reaction, but rather the decoupling of solid particles from the polymer matrix. We will report on equation of state experiments conducted for epoxy, Al-SiO\(_2\) composites showing deviation from ideal Hugoniot behavior as a result of damage evolving at a critical impact stress. Two compositions prepared with significantly different volume fractions of polymer binder phase show damage occurring at approximately the same critical impact stress. The Burch-Murnaghan EOS is used to show the introduction of damage. Further validation of this effect is obtained from a constitutive model for tensile damage and distention (TDD) behavior available in the shock physics code, CTH.


Thursday, June 28, 2007 10:30AM - 12:30PM — Session P6 Reactive Materials II Fairmont Orchid Hotel Promenade I/II

10:30AM P6.00001 Effect of Aluminum Particle Size on the High Strain Properties of Pressed Aluminized Explosives, CHAD RUMCHIK, JENNIFER JORDAN, Air Force Research Laboratory — High strain rate mechanical properties of explosives are important in design as these materials see extreme loading environments. Previous studies have shown that decreasing the particle size of the explosive crystals in a PBX can increase the strength. In this study, pressed explosives (64% explosive, 30% aluminum, and 6% HTPB based binder) were prepared with varying aluminum particle size from 50 nm to 30+ µm in order to investigate the effect of aluminum particle size and morphology on the compressive stress-strain behavior of the material. The paper will present the experimental results of this study as well as an investigation into potential constitutive models for these materials.

10:45AM P6.00002 Detonation Failure Thickness Measurement in an Annular Geometry, DAVID B. MACK, OREN E. PETEL, ANDREW J. HIGGINS, McGill University — The failure thickness of neat nitromethane in aluminum confinement was measured using a novel experimental technique. The thickness was approximated in an annular geometry by the gap between a concentric aluminum tube and rod. This technique was motivated by the desire to have a periodic boundary condition in the direction orthogonal to the annulus thickness, rather than the free surface that occurs in a typical experiment in a rectangular prism geometry. This results in a two-dimensional charge analogues to previous failure thickness setups but with infinite effective width (i.e. infinite aspect ratio). Detonation propagation or failure was determined by the observation of failure patterns engraved on the aluminum rod by the passing detonation. Analysis of these engraved patterns provides a statistical measurement of the spatial density of failure waves as the failure thickness is approached. The failure thickness was measured to be 0.76 mm ± 0.25 mm, which agrees with previous results, obtained using a rectangular prism geometry.

11:00AM P6.00003 Simulation of Particle Size Effect on Dynamic Properties and Fracture of PTFE-W-Al Composites, ERIC HERBOLD, Dept. of Mechanical and Aerospace Engineering, University of California, San Diego, La Jolla, CA 92093-0411, JING CAI, Materials Science and Engineering Program, University of California, San Diego, La Jolla, CA 92093-0418, DAVID BENSON, VITALI NESTERENKO, Dept. of Mechanical and Aerospace Engineering, University of California, San Diego, La Jolla, CA 92093-0411 — Recent investigations of the dynamic compressive strength of cold isostatically pressed (CIP) composites of polytetrafluoroethylene (PTFE), tungsten and aluminum powders show significant differences depending on the size of metallic particles. PTFE and aluminum mixtures are known to be energetic under dynamic and thermal loading. The addition of tungsten increases density and overall strength of the sample. Multi-material Eulerian and arbitrary Lagrangian-Eulerian methods were used for the deformation and fracture of tungsten-PTFE mixtures. We present measurements of the release of alpha quartz into SiO\(_2\) aerogel whose EOS had been calibrated by direct measurements. The calculations indicate that the observed dependence of sample strength on particle size is due to the formation of force chains under dynamic loading in samples with small particle sizes even at larger porosity in comparison with samples with large grain size and larger density.

3This research was supported by the ONR award N00014-06-1-0263

11:15AM P6.00004 High-Speed Photography of Detonation Propagation in Dynamically Pre-compressed Liquid Explosives, OREN PETEL, ANDREW HIGGINS, McGill University, AKIO YOSHINAKA, FAN ZHANG, DRDC Suffield — The propagation of detonation in shock compressed nitromethane was observed with a high speed framing camera. The test explosive, nitromethane, was compressed by a reverberating shock wave to pressures on the order of 10 GPa prior to being detonated by a secondary detonation event. The pressure and density in the test explosive prior to detonation was determined using two methods: manganin strain gauge measurements and LS-DYNA simulations. The pressure and density of the wave was found to depend very weakly on strength of confinement, but more strongly on packing density. Traditional detonation mechanisms such as volume expansion and front curvature may consequently not be applicable in systems with solid reactants and products. Post-test examination of the charges showed nearly complete reaction of the powder in most cases, indicating a sustained reaction in spite of the decay of the supersonic part of the reaction.

11:30AM P6.00005 Shock-induced reaction in Ti-Si powder mixtures, JULIAN LEE, FAN ZHANG, DRDC Suffield — The reactive properties of shocked powders consisting of a mixture of titanium and silicon have been investigated experimentally in cylindrical charges initiated by high explosives. Selected tests using a flyer plate for initiation were also performed for comparison. Although titanium and silicon are known to degrade and produce high-temperature solid products, shock-initiated reactions are not yet understood. We will report on equation of state experiments conducted for epoxy, Al-SiO\(_2\) composites showing deviation from ideal Hugoniot behavior as a result of damage evolving at a critical impact stress. Two compositions prepared with significantly different volume fractions of polymer binder phase show damage occurring at approximately the same critical impact stress. The Burch-Murnaghan EOS is used to show the introduction of damage. Further validation of this effect is obtained from a constitutive model for tensile damage and distention (TDD) behavior available in the shock physics code, CTH.
11:45AM P6.00006 Mechanical and Microstructural Properties of PTFE/Al/W Composite

JING CAI, FENGCHUN JANG, KENNETH VECCHIO, MARC MEYERS, VITALI NESTERENKO, University of California, San Diego — Mechanical and microstructural properties of PTFE/Al/W composites with a density up to 7.1 g/cc fabricated by cold isostatic pressing with identical weight ratios of constituents (PTFE serving as the matrix) were investigated using quasi-static and Hopkinson Bar compression tests. The ultimate compressive strengths of the PTFE/Al/W composite (7.1 g/cc) with coarse W particles was ~18 MPa (quasi-static loading) and ~24 MPa (dynamic loading), while more porous PTFE/Al/W composite with fine W particles (5.9 g/cc) had flow stress 24 MPa (quasi-static) and 44 MPa (dynamic). Critical strains to failure for both composites are 4.5%. We attribute this unusual behavior to force chains created by small tungsten particles. Environmental scanning electron microscope revealed that the PTFE matrix was populated by a homogeneous distribution of nanocracks and nanofibers of PTFE were observed after drop-weight tests.

2This research was supported by ONR, Award No: N00014-06-1-0263.

12:00PM P6.00007 Impact Initiation of Rods of Pressed Polytetrafluoroethylene (PTFE) and Aluminum Powders

WILLIS MOCK, JR., JASON T. DROTAR, Naval Surface Warfare Center, Dahlgren — A gas gun has been used to investigate the impact initiation of rods consisting of a mixture of 72 wt% PTFE (28 µm particle size) and 28 wt% aluminum (95 micron particle size) powders. The rods were 7.6 mm in diameter by 51 mm long, and were fabricated from material that had been pressed and sintered to a full density of 2.27 gm/cm³. They were sabot-launched into steel anvils at impact velocities ranging from 468 to 970 m/sec. This corresponds to calculated initial impact stresses of 25 to 64 kbar, respectively. A framing camera was used to observe the time sequence of events. These include change in rod shape, fracture, and the initiation and evolution of the reaction phenomena. The time of observation of first light after impact was taken as the initiation time. Initiation occurred at discrete locations in the impacted material. At the lowest impact stress of 25 kbar no light was observed; this value was taken as the initiation threshold stress for this material. Above the initiation threshold, the initiation time dropped abruptly from 74 µs at just above threshold to 14 µs at the highest impact velocity of 970 m/s. These results are compared with rod impact experiments for a similar material in which the only major difference is a smaller aluminum particle size (9 micron).

11:15AM P7.00004 Detonation propagation in high explosives

LINHBAO TRAN, US Army Research Laboratory — Detonation wave modeled as a Chapman-Jouquet detonation using a hydrodynamic burn is investigated. Detonation front is represented by a level-set function and its propagating velocity is calculated through the Hugoniot jump conditions in local shock coordinate. Conservation laws are solved for both gas and solid phase with full coupling applied at material interfaces. Boundary conditions at free surfaces as well as solid surfaces are accurately handled. Validation is performed for a PBX-9501 cylinder. Simulation of detonation propagating through a bed of Aluminum particles show a complex flow field behind the detonation with multiple shock-shock interactions, as well as a slowed down detonation wave. Corner turning problem is also performed and compared with other numerical and experimental results.

12:15PM P6.00008 Reaction of Titanium and Zirconium Particles in Cylindrical Explosive Charges

DAVID FROST, MALCOLM CAIRNS, SAMUEL GOROSHIN, McGill University, FAN ZHANG, DRDC-Suffield — The critical conditions for the initiation threshold, the initiation time dropped abruptly from 74 µs at just above threshold to 14 µs at the highest impact velocity of 970 m/s. These results are compared with rod impact experiments for a similar material in which the only major difference is a smaller aluminum particle size (9 micron). [1] W. Mock, Jr. and W. H. Holt, in Proc. APS Shock Compression of Condensed Matter–2005, p.1097.

Thursday, June 28, 2007 10:30AM - 12:15PM

Session P7 Detonation Shock Dynamics
Fairmont Orchid Hotel Promenade III

10:30AM P7.00001 Detonation Shock Dynamics Calibration of PBX 9501
TARIQ ASLAM, Los Alamos National Laboratory — Detonation shock dynamics (DSD) has proven to be a fast and accurate alternative to direct numerical simulation of propagating detonations. Here, the requisite differential equations, experimental data and calibration procedure will be outlined for the plastic bonded explosive PBX 9501. It will be shown that the DSD model can fit the existing PBX 9501 data to within the experimental uncertainty.

10:45AM P7.00002 Application of Detonation Shock Dynamics (DSD) on Youngs-Type Discontinuous Interface Geometry
TORU AIDA, JOHN WALTER, Los Alamos National Laboratory — Detonation Shock Dynamics (DSD) describes the evolution of two- or three-dimensional detonation wave by assuming that the detonation reaction zone is significantly small and that the curvature of the detonation wave front is also small with respect to the explosive in question. The current DSD solver obtains its input parameters by superimposing (normally rectangular Cartesian) grid points over the high explosive regions, having assigned distances from each grid point to the HE boundaries (+: inside of HE; -: outside) and assigning material identification to each grid point based on its location within the system. It has been shown to work with Lagrangian mesh where mesh entities, particularly cell faces, are contiguous and therefore, distances to material interfaces, namely HE and other materials and/or external boundaries, are precisely defined. In this paper a new scheme of DSD driver code to allow the material interfaces to be expressed in a discontinuous manner, such as Youngs material interface construction for 3D Eulerian hydrodynamics code.

11:00AM P7.00003 An extension of detonation shock dynamics for insensitive explosives
MARK SHORT, JOHN BDZIL, TARIQ ASLAM, LANL — Resolved, direct numerical simulations of the detonation of high explosives (HE) in geometries of engineering interest are largely unattainable due to the scale disparity between the shorter detonation reaction-zone length and the longer characteristic explosive charge dimension. However, multi-scale mathematical modeling, utilizing this scale disparity, has led to the development of the theory of detonation shock dynamics (or DSD). With DSD, the propagation of a detonation in a HE configuration is described by a surface evolution equation for the detonation front. For insensitive high explosives (IHE), detonations typically have two characteristic reaction stages: a fast reaction where the majority of the heat of reaction is released, followed by a second significantly slower reaction (e.g. from carbon coagulation in PBX-9502). We show that the presence of this slowly reacting, weak heat release zone can have a significant (time-dependent) influence on the evolution of a detonation in IHE. We also describe an extension to the DSD concept, specifically tailored to detonations, in IHE which treats fast-slow chemistry models. The fast chemistry is handled with a DSD front rationally coupled to a distributed, resolved (reactive burn) model for handling the slow chemistry step.

11:15AM P7.00004 Detonation propagation in high explosives
LINHBAO TRAN, US Army Research Laboratory — Detonation wave modeled as a Chapman-Jouquet detonation using a hydrodynamic burn is investigated. Detonation front is represented by a level-set function and its propagating velocity is calculated through the Hugoniot jump conditions in local shock coordinate. Conservation laws are solved for both gas and solid phase with full coupling applied at material interfaces. Boundary conditions at free surfaces as well as solid surfaces are accurately handled. Validation is performed for a PBX-9501 cylinder. Simulation of detonation propagating through a bed of Aluminum particles show a complex flow field behind the detonation with multiple shock-shock interactions, as well as a slowed down detonation wave. Corner turning problem is also performed and compared with other numerical and experimental results.
11:30AM P7.00005 Critical Ignition Transients in Condensed Explosives, D. SCOTT STEWART, SUNHEE YOO, University of Illinois, DAVID E. LAMBERT, Air Force Research Laboratory, Munition Directorate — Comparisons of the motion of a detonation shock measured in experiment, that predicted by the asymptotic theory of detonation shock dynamic (DSD-theory) that include shock acceleration, and direct multi-material simulation are made. A non-ideal, reactive equation of state and a rate law is used to describe the explosive and was employed in both the theoretical (DSD) calculations and the multi-material simulations. The experiment, theory are found to be in excellent agreement and this indicates that for a large class of important detonation flows one can apply the DSD model. DSD assumes that the detonation shock propagates along its normal direction with its speed determined by its total shock curvature (D-kappa). We present a calculation of critical energies and initial conditions needed to light the explosive using theory and show comparison with experiments conducted by Lambert in HMX-based explosives.

11:45AM P7.00006 Detonation Failure in Ideal and Non-Ideal Explosives, P.J. HASKINS, M.D. COOK — In this paper we revisit and extend the classic treatment of detonation failure developed by Eyring et. al. [1]. We recently published a development of this theory [2] in which a pressure dependant rate law was substituted for the Arrhenius temperature dependant law originally considered. Here we show that by assuming a 2-component rate law based upon a temperature dependant ignition phase and a pressure dependant growth phase we are able to rationalise the very different failure characteristics (critical diameter and velocity decrement at failure) of ideal and non-ideal explosives.


12:00PM P7.00007 Physical Model of Low Velocity Detonation in Plasticized HMX, KONSTANTIN GREELEN, KNITFF, MICHAIL TARIKIN, SVETLANA TSARENOVA, ALEXANDER SHITIKO — Phenomenon of low velocity detonation (LVD) is known for many years, but its physical mechanism has not been understood in details, yet. A physical model of LVD is presented in the given report. The main idea of the model is that LVD in dense plasticized explosives may take place only when due to the lateral unloading the pressure at the leading shock front is reduced as compared to that at normal detonation (ND). As a result, the chemical reaction rate and, hence, the energy released between the leading shock front and the sound surface must be lesser as compared to that at ND. But, from other side, this may be enough to sustain the stationary regime of the LVD propagation. The model has been implemented in 2-D hydrocode and verified by means of computer modeling of the experiments (Leuret e.a., 1998) where LVD was observed in plasticized HMX. The results of our calculations supports the suggestion that LVD wave in plasticized HMX is a complex of the leading shock wave having pressure near 1 GPa and the compression wave following the front. Stationary propagation of such structure is possible only when some specific combination of the energy release rate and the lateral unloading intensity takes place.

Thursday, June 28, 2007 1:45PM - 3:15PM —
Session Q2 First Principles and Molecular Dynamics Calculations IV Fairmont Orchid Hotel Amphitheater

1:45PM Q2.00001 Dynamics of Plastic Deformation in Atomic Shock Compression Simulations, WILHELM WOLFEN, ALISON KUBOTA, Lawrence Livermore National Laboratory — Dynamics simulations of shock compression of aluminum are evaluated in terms of a continuum mechanics descriptions to obtain detailed stress and strain distributions behind shock fronts. The equivalent or von Mises stress reaches steady values that coincide with the dynamic yield strength obtained by Huang and Asay from the analysis of particle velocity profiles of release and reshock experiments. This agreement is all the more significant as the experimental results are indirect, while the atomistic simulation results extract the dynamic strength directly. Additional information is obtained when the evolution of the von Mises stress is viewed in the Lagrangian frame. Different material elements experience nearly the same stress evolution: a rapid rise, as the elastic wave front passes the material element, followed by an exponential decline of the von Mises stress. This evolution implies a constitutive law for plastic deformation that can be used as in finite element codes, and/or it can be further interpreted by the dislocation mechanisms that the atomistic simulations so vividly reveal and display. Temperature can also be extracted directly from the atomistic simulations and be separated into adiabatic and plastic heating.

2:00PM Q2.00002 Frictional interactions at compressed Al interfaces, J.E. HAMMERBERG, Los Alamos National Laboratory, R. RAVELO, University of Texas, El Paso, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — We discuss the velocity and temperature dependence of the frictional force at sliding Al-Al interfaces. A series of 3-D 1.5 million atom Non Equilibrium Molecular Dynamics (NEMD) simulations for single crystal Al incommensurate interfaces have been carried out and apply it shock compression of single-crystal Aluminum using very large-scale atomistic wave-propagation simulations. In the first part of this presentation, we discuss the performance of the available and newly developed interatomic potentials in terms of their ability to reproduce thermoelastic and plastic properties such as elastic moduli, specific heat, thermal expansion coefficient, thermal conductivity and gamma surface. We then describe recent large-scale simulations of ramp- and cyclically-loaded single-crystal Aluminum with varying initial defect concentrations. Using the method of characteristics, we impose a time-varying longitudinal force to generate ramp waves with specified shock-up locations in the material. Our calculations demonstrate that (1) the initial defect densities have a strong effect on the time-dependence and the maximum achieved equivalent stress, (2) shock-up consistently occurs earlier than expected due to the inherent inability for materials to sustain large gradients in the shock front at these micron length-scales, and that (3) the observed flow stress followed in the coarse-grained Lagrangian elements before shock-up are consistently higher than those after shock-up and those from shock-loading simulations. We discuss these differences in terms of continuum phenomenological models for plastic deformation constructed from coarse-grained analyses of these simulations, and consider future possible developments in large-scale atomistic simulations.

2:15PM Q2.00003 Single Crystal Plasticity in Ramp- and Cyclically-Loaded Aluminum, ALISON KUBOTA, Lawrence Livermore National Laboratory — In recent years, there has been a great deal of interest in using large-scale atomistic simulations to model wave propagation in order to get a qualitative picture for inelastic deformation in materials. Although these simulations have provided a great deal of qualitative insight into the phenomena of high strain rate deformation in materials, there is an increasing need to be able to obtain quantitative continuum descriptions for the atomistic simulations in terms of stresses and strains so one can construct constitutive laws for plastic deformation. This presentation will be focused on recent work to develop this seamless approach from atoms to continuum and apply it shock compression of single-crystal Aluminum using very large-scale atomistic wave-propagation simulations. In the first part of this presentation, we discuss the performance of the available and newly developed interatomic potentials in terms of their ability to reproduce thermoelastic and plastic properties such as elastic moduli, specific heat, thermal expansion coefficient, thermal conductivity and gamma surface. We then describe recent large-scale simulations of ramp- and cyclically-loaded single-crystal Aluminum with varying initial defect concentrations. Using the method of characteristics, we impose a time-varying longitudinal force to generate ramp waves with specified shock-up locations in the material. Our calculations demonstrate that (1) the initial defect densities have a strong effect on the time-dependence and the maximum achieved equivalent stress, (2) shock-up consistently occurs earlier than expected due to the inherent inability for materials to sustain large gradients in the shock front at these micron length-scales, and that (3) the observed flow stress followed in the coarse-grained Lagrangian elements before shock-up are consistently higher than those after shock-up and those from shock-loading simulations. We discuss these differences in terms of continuum phenomenological models for plastic deformation constructed from coarse-grained analyses of these simulations, and consider future possible developments in large-scale atomistic simulations.

1This work was performed under the auspices of the US Department of Energy by the University of California Lawrence Livermore National Laboratory under contract W-7405-Eng-48.

2This work was performed under the auspices of the US Department of Energy by the University of California Lawrence Livermore National Laboratory under contract W-7405-Eng-48.
2:45PM Q2.00004 Liquid Metal Free Energies from Ab Initio Potential Surfaces, CARL GREEFF, RAQUEL LIZARRAGA, ERIC CHISOLM, Los Alamos National Laboratory — For prediction of high pressure melting curves and liquid thermodynamic properties, it is desirable to evaluate liquid free energies. Direct free energy calculations from *ab initio* potential surfaces are very computationally intensive, especially for transition metals. Here we investigate Monte Carlo methods that involve sampling on the surface defined by a reference system. In principle, this allows for large gains in efficiency because the random walk is carried out on the (much faster) reference potential, and the *ab initio* potential is only evaluated on a small subset of uncorrelated configurations. We investigate the feasibility of these methods, and the role of the reference system. Results will be presented for liquid Mg and Ta.

3:00PM Q2.00005 Quantum Molecular Dynamics Simulations of Optical Reflectivity of Shock-Compressed Tin, JOEL KRESS, LEE COLLINS, Los Alamos National Laboratory, STEPHANE MAZERET, CEA/DAM — Shock-compression experiments have measured the optical reflectivity of tin to detect: (1) a solid-solid phase transition (J → BCT); (2) melting on the Hugoniot curve, and; (3) melting during the release of the strongly shocked material. Recent quantum molecular dynamics (QMD) simulations have been successful at determining the optical properties of warm, dense materials such as shock-compressed deuterium, exploding wires made of aluminum and copper, and laser-heated thin films of gold. In this work, we present QMD calculations of the optical conductivity and reflectivity of solid (cold) β-tin, representative of shock-compressed and shock-released states. Calculated differences in the optical reflectivity between the cold and warm states will be compared with the measurements from shock-compressed experiments.

**Thursday, June 28, 2007 1:45PM - 3:45PM — Session Q3 Isentropic and Off Hugoniot Loading II**
Fairmont Orchid Hotel Plaza I

1:45PM Q3.00001 Compressive strength of aluminum under high-rate loading, JAMES ASAY, Sandia National Laboratories — The compressive yield strength of materials is important in a number of scientific and applied applications. Techniques for measuring strength at high pressure are limited, with the result that measurements have been made on only a few materials. Shock and quasi-isentropic loading are important techniques for studying material strength and other properties over a broad range of initial loading rates and high stresses. The combined use of these techniques on a single material allows evaluation of the history dependence of strength properties, including effects of loading history, pressure, and temperature. Wave profile methods for estimating strength properties have been applied to a systematic study of the compressive strength of aluminum for a variety of initial material properties, loading rates, peak stress, and for cyclic loading. I will present recent wave profile measurements of yield strength in several aluminum alloys using these different techniques. The combined data reveal several observations about history effects of the yield strength in aluminum, including a general increase with longitudinal stress and an insensitivity to initial metallurgical properties for both shock and quasi-isentropic loading. In particular, the results suggest that deformation processes produced in both processes appear to have a larger effect than initial material properties on the change in strength at high pressure. In addition, it is found from cyclic loading experiments that pressure appears to be the dominant hardening mechanism in aluminum at high rates and high pressures.

2:15PM Q3.00002 Material Strength on Quasi-isentropes, JEFFREY H. NGUYEN, J. REED PATTERSON, DANIEL ORLIKOWSKI, L. PETER MARTIN, NEIL C. HOLMES, Lawrence Livermore National Laboratory — We have recently carried out off-Hugoniot dynamic compression experiments on aluminum to gain insight into its yield strength. The samples were initially shocked to a fixed state on the Hugoniot, then quasi-isentropically compressed and released isentropically. We designed the functionally graded density impactor (FGDI) such that the strain rates on compression and release isentropes are nearly equivalent. Here, we will discuss the details of the experiments and error analysis in deriving the yield strength of aluminum on a "hot" quasi-isentrope. We will also discuss recent advances in the FGDI technology that made these experiments possible with significantly reduced uncertainties. Methods to characterize these advances will be discussed. Work performed under the auspices of the U.S. DOE at the University of California/Lawrence Livermore National Laboratory under contract W-7405-ENG-48.

2:30PM Q3.00003 Ramp Compression of Diamond to Over 1000 GPa, JON EGGERT, DAVID BRADLEY, PETER CELLIERS, GILBERT COLLINS, DAMIEN HICKS, DAVID BRAUN, SHON PRISBREY, RAY SMITH, Lawrence Livermore National Laboratory, THOMAS BOEHLY, University of Rochester — Isentropic compression of materials to multi-megabar pressures has long been a grand challenge for high-density and planetary science. Recently, ramp-wave experiments have demonstrated quasi-isentropic compression using lasers, pulsed-power, and impactors with peak pressures up to 240 GPa[1,2]. Using a tailored-radiation drive at the Omega laser we have ramp-compressed and measured the stress-strain relation in diamond to over 1000 GPa, more than 4 times the maximum previously attained. We find an elastic-plastic transition at 60-70 GPa in good agreement with the elastic and release isentropes are nearly equivalent. Here, we will discuss the details of the experiments and error analysis in deriving the yield strength of aluminum on a "hot" quasi-isentrope. We will also discuss recent advances in the FGDI technology that made these experiments possible with significantly reduced uncertainties. Methods to characterize these advances will be discussed. Work performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No. DE-AC04-94AL85000.

2:45PM Q3.00004 Interaction of Material Strength With Ramp and Shock Wave Loading, JOW-LIAN DING, Washington State University, JAMES ASAY, Sandia National Laboratories — The objective of the current study is to gain a detailed understanding of the interaction of the material strength with the ramp and shock wave loadings. The ultimate goal is to use the foundation established in this study to develop a practical methodology to extract strength information from ramp and shock wave experiments. A forward, numerical-simulation-based understanding of the interaction of the material strength with the ramp and shock wave loadings is potentially a very effective tool to probe the rate sensitivity of material strength.
3:00PM Q3.00005 Dynamic Response of Kovar to Shock and Ramp-Wave Compression. 1

J.L. WISE, S.C. JONES, C.A. HALL, J.R. ASAY, D.M. SANCHEZ, Sandia National Laboratories — Complementary gas-gun and electromagnetic pulse tests conducted in Sandia’s Dynamic Integrated Compression Experimental (DICE) Facility have, respectively, probed the behavior of electronic-grade Kovar samples under controlled impact and intermediate-strain-rate ICE (Isentropic Compression Experiment) loading. In all tests, velocity interferometer (VISAR) diagnostics provided time-resolved measurements of sample response for conditions involving one-dimensional (i.e., uniaxial strain) compression and release. Wave-profile data from the gas-gun impact experiments have been analyzed to assess the Hugoniot Elastic Limit (HEL), Hugoniot equation of state, spall strength, and high-pressure yield strength of shocked Kovar. The ICE wave-profile data have been interpreted to determine the locus of isentropic stress-strain states generated in Kovar for deformation rates substantially lower than those associated with a shock process. The impact and ICE results have been compared to examine the influence of loading rate on high-pressure strength.

Ktech Corporation, Albuquerque, NM 87123-3336

Contract DE-AC04-94AL85000.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

3:15PM Q3.00006 Strength Measurements of Dry Indiana Limestone using Ramp Loading Techniques1

BILL REINHART, TRACY VOGLER, LALIT CHHABILDAS, Sandia National Laboratories — One of the most accurate methods to control strain rates in dynamic compressions studies makes use of the non-linear elastic property of glass to transform an initial shock into a ramp wave of know amplitude and duration. Fused silica is calibrated for this purpose and when placed between the limestone specimen and the projectile, strain rates in the range of 10^3/s can be achieved. Ramp loading strain rates are higher than what can be produced on Hopkinson bars and lower than what shock experiments attain. Ramp wave compression tests have been performed on dry Indiana limestone at strain rates of approximately 3 x 10^3/s. The strength determined at the elastic under ramp loading is consistent with Hopkinson bar measurements and shows a significant strength increase with increasing strain rate.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

3:30PM Q3.00007 Two-step loading in a Split Hopkinson Pressure Bar (SHPB) at different strain rates

RACHEL BRIGGS, DAVID WILLIAMSON, DANIEL DRodge, WILLIAM PROUD, University of Cambridge — In conventional Split Hopkinson Pressure Bar (SHPB) testing the striker bar is single-piece and made of the same material as the input- and output-bars. When the striker-bar strikes the input-bar the resulting top-hat stress profile travels down the input-bar and the sample is loaded at a strain-rate related to the magnitude of that top-hat stress. (Actually, strain and strain-rate are calculated from the reflected wave). Here we show results from a system that uses a composite striker-bar formed from two equal lengths of materials with different mechanical impedances. When the composite striker-bar strikes the input-bar the result is a two-step stress profile. Correspondingly, the sample is consecutively loaded at two different strain-rates. This can be a low strain-rate followed by a higher strain-rate, if the low impedance element is first incident on the input-bar, or vice versa. The major benefit of this method is that the sample does not experience repeat loading or significant unloading between the two regimes. This paper outlines the current state of research and details show reasonable agreement. Details describing the computational methods used in these simulations will be discussed.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. Department of Energy under Contract No. DE-AC04-94AL85000.

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Thursday, June 28, 2007 1:45PM - 4:00PM
Session Q4 Experimental Developments IV Fairmont Orchid Hotel Plaza II

1:45PM Q4.00001 3D Simulation Capability for Isentropic Compression Loads

S. CHANTRENNE, T. AO, J.R. ASAY, T.A. HAILL, H.L. HANSHAW, C.A. HALL, Sandia National Laboratory — For the past 10 years, equation-of-state experiments have been carried out using magnetic pressure to isentropically compress materials. Recently, a compact, fast strip-line pulser was designed with the objective of doing isentropic compression experiments at low cost, with rapid turn around, with good shot-to-shot reproducibility, and with the ability to shape the current profile for the material being tested. In this work, we present the results of 3D simulations of isentropic compression loads that were performed with Sandia National Laboratories\' ALEGRA MHD code. In order to understand the pressure magnitude and uniformity, current density distributions were calculated from the capacitors to the load. Free-surface velocity measurements are compared to those obtained from these simulations and show reasonable agreement. Details describing the computational methods used in these simulations will be discussed.

2:00PM Q4.00002 Development of a Single Stage Implosion-Driven Hypervelocity Launcher

DANIEL SZIRTI, JASON LOISEAU, PATRICK BATCHELOR, ANDREW HIGGINS, VINCENT TANGUAY, FAN ZHANG, McGill University — Work carried out on the development of a single stage implosion-driven hypervelocity launcher is presented. Explosives surrounding a thin-walled tube filled with helium works similar to the pump tube of a conventional light gas gun. Implosion of the tube drives a strong shock that reflects back and forth between the projectile and the implosion pinch, generating very high temperatures and pressures. Experiments to evaluate the implosion dynamics and performance of the pump tube were carried out, with attention given to the helium fill pressure, diameter of the pump tube, thickness of the explosive layer, and the presence of a tamper. Simple analytic models were used to approximate the performance of the launcher; their advantages and limitations are discussed. Experiments with an implosion-driven launcher demonstrated muzzle velocities of 4 km/s with 4-mm-diameter aluminum projectiles, giving good agreement with the analytical models of performance. Projectile integrity was verified by high-speed photography and other diagnostics.

2:15PM Q4.00003 Modeling of an Implosion Driven Hypervelocity Launcher

JASON LOISEAU, ANDREW HIGGINS, DANIEL SZIRTI, PATRICK BATCHELOR, McGill University, FAN ZHANG, DRDC Suffield, VINCENT TANGUAY, DRDC Valcartier — Modelling work carried out on the implosion driven launcher under concurrent development is presented. The launcher consists of a thin walled metal tube surrounded by explosive which when detonated pinches the tube shut and drives a strong shock into the projectile. The commercial hydrocode LS-DYNA was used to quantitatively and qualitatively evaluate the design parameters of the launcher and their effect on implosion dynamics and performance. These parameters include fill pressure, tube diameter, explosive layer thickness, and explosives tampering. The launcher is primarily modeled using a quasi 2D Arbitrary Langrage Euler formulation. A full 3-D axisymmetric model is also employed. The model is evaluated against experimental data previously collected. Additional developmental work on a second stage launcher taking advantage of a phase velocity between the imploding tube and explosives via the use of angled flyer plates and cones is also carried out.
using the simulant sucrose. Discrete crystal plasticity we have begun nano-indentation experiments on the crystals demonstrating plastic yielding without fracture in RDX, a technique tested in the elastic-plastic transition as observed in randomly oriented powders or perhaps sufficiently defective single crystals. To understand the relative importance of probe microscopy. In previous experiments on (100) oriented crystals, multiple elastic peaks were thought to be due to cracks in specific directions introduced with Monte Carlo calculations performed using a TIP4P potential. In collaboration with Kyle Ramos, Los Alamos National Laboratory and David Bahr, Washington State University.
2:15PM Q6.00002 A Study of the Shock Sensitivity of PBX 9501 Damaged by Compressive Loading, DARLA THOMPSON, RICHARD GUSTAVSEN, DANIEL HOOKS, PAUL PETERSON, RACCI DELUCA, DAVID STAHL, STEPHANIE HAGELBERG, Los Alamos National Laboratory, ROBERT ALCON, DE DIVISION, LANL TEAM — We have studied the effects of damage caused by compressive loading on the shock sensitivity of the plastic bonded explosive PBX 9501. PBX 9501 consists of 95 wt. % HMX (C4H8N8O8) and 5 wt. % Nitropolyesteric Ectane binder. The binder is a mixture of 49 wt. % Ectane®7503 (BF Goodrich), 49 wt. % Nitroplasticizer (a 50/50 eutectic mixture of bis(2,2-dinitropropyl)formal and bis(2,2 dinitropropyl)acetal), and 2 wt. % Irganox® 1010 stabilizer. PBX 9501 cubes, 25.4 mm on a side, were subjected to various uniaxial compressive loads in an Instron machine. After loading, 3.5 mm thick slices were taken from the center of each cube. These slices were then subjected to nearly identical 35 kbar shocks. Transmitted shock wave profiles were measured using interface velocimetry (VISAR). Comparison of shock wave growth is a measure of shock sensitivity. Results on four specimens are being analyzed relative to previous baseline data on PBX 9501 at various pressed densities, to determine if the response of damaged material is due to factors other than simple density changes. (LA-UR 07-1256)

2:30PM Q6.00003 High Strain, Strain Rate Behavior of PTFE/Al/W1. JOHN ADDISS, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK, JING CAI, Materials Science and Engineering Program, University of California San Diego, CA 92093, STEVE WALLACE, WILLIAM PROUD, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK, VITALI NESTERENKO, Department of Mechanical and Aerospace Engineering, University of California San Diego, CA 92093 — Conventional droptweight technique was modified to accommodate low amplitude signals from low strength, cold isostatically pressed energetic “heavy” composites of polytetrafluoroethylene (PTFE)/Al/W. The friction strength, strain and post-critical behaviour of fractured samples were measured for samples of different porosity and W grain size (the masses of each component being the same in each case). Unusual phenomenon of significantly higher strength (55 MPa) of porous composites (density 5.9 g/cc) with small tungsten particles (1 micron) in comparison with strength (32 MPa) of dense composites (7.1 g/cc) with larger tungsten particles (20 micron) was observed. This is attributed to force chains created by a network of small tungsten particles. Interrupted tests at the different level of strains revealed mechanism of fracture under dynamic compression.

2:45PM Q6.00004 Shear Induced Reaction Localizations and Mechanisms of Energy Dissipation in PBX Subjected to Strong Shock1, IGOR PLAKSIN, LEDAP-Lab of Energetics and Detonics, Univ. of Coimbra — Paper addresses two emerging topics: how reaction initiation arises when PBX is subjected to shock and how detonation wave becomes oscillating. We apply the 96-channel analyzer for simultaneous measurements of radiation from the reaction spots surface and stress field caused by shock or detonation reaction zone in multi-layer optical monitor. This metrology allows meso-scale probing of the 3-D structure of shock- or detonation- reaction-zone as well as revealing mechanisms of its formation at different initiation scenarios. The dominant role of the shear driven plastic deformation in initiation scenario is disclosed in all tested PBX-s (including simulants of PBXN-110, PBAN-128, PBXN-109, 111, 121 and B-2208), in wide range of PBX sample sizes: from 1 mm3 (single crystal within the binder) up to few cm3. This research is complementing a separate, longer running, theoretical effort by Dr. Steve Coffey that examines the solid-state quantum physics responsible for initiation of explosive crystals subjected to shock or impact. Finally, this represents a novel research effort to relate plastic deformation, energy dissipation and localization in crystals to shear and shear deformation. The accompanying experimental results strongly support Coffey’s theoretical prediction that initiation is due to shear driven plastic deformation and is not due solely to uniform shock pressure. Finally, we will present and discuss the recently revealed phenomenon of the detonation mechanisms and the formation of shockinduced reaction zone in PBX subjected to strong shock.

3:15PM Q6.00005 A Viscoelastic Fracture Model for Simulation of Solid Propellant Impacts, ERIK R. MATHESON, Lockheed Martin Corporation — A viscoelastic kinetics (VEK) model for deformation and damage in solid rocket propellant has been previously developed and correlated to an extensive set of experimental data to determine mechanical properties. Ultimately, VEK will be extended to perform coupled damage and reaction modeling of DXT during propellant impacts. There are two types of damage considered in VEK: 1) decohesion at particle/binder interfaces, and 2) scission of the binder. The first type of damage leads to formation of essentially spherical voids around the decohered particles, and development of a model for the surface area that supports combustion is rather straightforward. The second type of damage leads to formation of propellant rubble, and the fineness depends on the impact stresses. Thus, a kinetic fracture model describing surface area generation due to scission damage has been added to the VEK model. To obtain data on the surface area generated, 25 mm L/D=1 propellant samples were fired into steel target plates at various velocities, and the resultant fragments were collected and burned in a combustion bomb. The total surface area generated was then estimated for each impacted sample. The upgraded VEK model is used to simulate the 25 mm impact experiments and is correlated to the combustion bomb data. This work was supported by NSWC-IH under the purchase order N00174-05-M-0085.

Thursday, June 28, 2007 1:45PM - 3:00PM — Session Q7 Post Detonation Effects Fairmont Orchid Hotel Promenade III

1:45PM Q7.00001 Factors Affecting Internal Blast1, RICHARD GRANHOLM, HAROLD SANDUSKY, JOSHUA FELTS, NAVSEA Indian Head — Internal blast refers to explosion effects in confined spaces, which are dominated by the heat output of the explosive. Theoretical temperatures and pressures may not be reached due to heat losses and incomplete gas mixing. Gas mixing can have the largest effect, potentially reducing peak quasi-static pressure by a factor of two due to lack of thermal equilibrium between products and atmosphere in the space, without including the incomplete combustion of excess fuel when the atmosphere is air. Chamber and test geometry affect gas mixing, which has been inferred through a number of experimental techniques and compared to calculations, for both large- and small-scale tests. Observations of late-time combustion depend on the extent of mixing and whether the excess fuel is gaseous or aluminum particles.

2:00PM Q7.00002 Cylindrical Explosive Dispersal of Metal Particles, R.C. RIPLEY, L. DONAHUE, Martec Ltd. Y. HORIE, C.M. JENKINS, AFRL, F. ZHANG, DRDC Suffield — The explosive dispersal of densely-packed metal particles in cylindrical RDX-based charges is studied numerically. Simulations are conducted with a reactive multiphase fluid-dynamic code. Spherical tungsten particles are applied in high metal mass fraction cylindrical charges in two configurations: a particle matrix uniformly embedded in a solid explosive versus an annular shell of particles surrounding a high-explosive core. The effect of particle number density is investigated by varying the nominal particle diameter from 27 to 120 μm while maintaining a constant metal mass fraction. Results are compared with steel particles to evaluate the influence of material density on dispersal. To account for early-time particle loading, momentum acceleration factors for shock interaction with packed metal particles are employed. The near-field dense granular heterogeneous flow effect is included in the governing equations and drag model; in the far-field, drag is the main driving force within the expanding detonation product gases and air. The dispersal dynamics are observed at radial locations in terms of arrival time, velocity and particle concentration. Results from experimental trials, described in the companion paper “Kinetic and Particle Characterization in Explosively-Driven Two-Phase Flow using PIV” by Jenkins et al., will ultimately be used to improve empirical-based drag models for dense supersonic multiphase flow.

1Supported by NSWC Indian Head core research program
2:15PM Q7.00003 Post-Detonation Energy Release from TNT-Aluminum Explosives, FAN ZHANG, JOHN ANDERSON, AKIO YOSHINAKA, DRDC Suffield, Canada — Detonation and post-detonation energy release from TNT and TNT-aluminum composite have been experimentally studied in an air-filled chamber, 26 m³ in volume and 3 m in diameter. While TNT has a high oxygen deficiency, experiments with 1.1 kg to 4 kg charges yield energy releases reaching only 86% of theoretical equilibrium values, possibly due to the non-uniform mixing between the detonation products and air. In order to improve mixing and further increase afterburning energy, large mass fractions of large aluminum particles are combined with TNT. The effect of particle distribution is also investigated in two composite configurations, whereby the aluminum particles are uniformly mixed in cast TNT or arranged in a shell surrounding a TNT cylinder. It is shown that the TNT-aluminum composite outperforms pure TNT, while improved performance is achieved for the shell configuration due to enhanced spatial mixing of hot fluids with oxidizing gases. Comparisons with the equilibrium theory and a liquid-based aluminized composite explosive (with an oxygen deficiency less than that of TNT) are conducted to further explore the mixing and afterburning mechanism.

2:30PM Q7.00004 Effect of shock compression on aluminum particle reaction in condensed media, AKIO YOSHINAKA, FAN ZHANG, DRDC Suffield — While it is known that aluminum particles, when mixed with an explosive, can react with detonation products and air, the effect that the detonation front has on the onset of aluminum reaction is not well understood. Past experiments have shown a dependence of particle reaction start time on confinement; reaction for 1-10 micronet particles occurs 1-10 microsec behind the detonation front. It is speculated that oxide layers are compromised by the detonation front and particle morphology changes significantly upon detonation passage. Of particular interest is the extent to which the presence and concentration of surrounding materials (e.g., binder, explosive, ... ) can influence the removal of the thin oxide layer encapsulating each particle. Samples consisting of aluminum powder tens of microns in diameter and mixed with an inert condensed phase additive were shock compressed through flyer plate impact to pressure levels comparable to those encountered during detonation (15-20 GPa). To confirm the extent to which particles react with detonation products, particle beds saturated with explosive were tested under similar conditions. Each sample, confined within a hermetically sealed test cell, was recovered after the experiment for microscopic analysis. The effects of particle size and particle-to-additive ratio were investigated as well.

2:45PM Q7.00005 Detailed Comparison of Blast Effects in Air and Vacuum, J.W. TRINGE, J.D. MOLITORIS, R.G. GARZA, H.G. ANDRESKI, J.D. BATTEUX, L.M. LAUDERBACH, E.R. VINCENT, B.M. WONG, Lawrence Livermore National Laboratory, ENERGETIC MATERIALS CENTER TEAM — We have performed a detailed investigation of blast effects from high-explosive detonations in air and in vacuum. This research was done with 4 kg charges in a large-volume fully contained spherical firing tank. The most obvious consequence of detonation in vacuum is that prompt shock effects are negated as the detonation has no external medium for coupling. The nature of the fireball is also completely altered due to the lack of surface combustion. However, we find that the net effect of the blast on large area witness plates is remarkably very similar in the air and vacuum environments. Diagnostics for this blast characterization included multiple-view high-speed imaging systems and time resolved pressure data gauges. Experimental results and model simulations will be presented.

Friday, June 29, 2007 8:00AM - 9:30AM – Session U2 First Principles and Molecular Dynamics Calculations V Fairmont Orchid Hotel Amphitheater

8:00AM U2.00001 Energetic materials under thermal shock: Molecular dynamics simulation with reactive force field, YI LIU, SERGEY ZYBIN, ADRI VAN DUIN, WILLIAM GODDARD, California Institute of Technology — The physical and chemical response of energetic materials under thermal shock loading has been investigated for RDX, PETN and HMX by molecular dynamics method with ReaxFF reactive force field parameterized from first-principles calculations. We study the propagation of a thermal front and following reactive wave from the hot spot created by fast heating of a local region and keeping it at high constant temperature. The hot spot serves as heat source to heat up adjacent materials where no temperature constraint is imposed, and trigger the chemical decomposition of energetic molecules. The mechanism and evolution of chemical reactions induced by thermal shock is discussed along with the propagation of heat, mass, pressure, and reaction waves. Acknowledgements: supported by ARO and ONR grants.

8:15AM U2.00002 Energetic materials under mechanical shock and shear: Molecular dynamics simulation with reactive force field, SERGEY ZYBIN, PENG XU, ADRI VAN DUIN, WILLIAM GODDARD, California Institute of Technology — The initial physical and chemical response of energetic materials under mechanical shock or shear loading has been investigated for RDX, PETN and HMX by molecular dynamics method with ReaxFF reactive force field parameterized from first-principles calculations. We study the propagation of a shock wave and shock-induced chemical reactions created by moving piston mimicked by a potential wall. We simulate both the continuous and impulsive loading to investigate its influence on the initiation and decomposition reactions in energetic materials as well as the orientational dependence using large-scale parallel ReaxFF-MD simulations. Besides, we perform a series of simulations of pure shear at high strain rate as well as static uniaxial compression of energetic crystals to study their transformation and decomposition under various loading conditions. The mechanism and evolution of chemical reactions induced by mechanical shock and pure shear is discussed along with the propagation of heat, mass, pressure, and reaction waves. Acknowledgements: supported by ARO and ONR grants.

8:30AM U2.00003 First-principles reactive molecular dynamics of initiation chemistry in energetic materials, AARON LANDERVILLE, IVAN OLEYNIK, University of South Florida, MORTKO KOZHUSHNER, Institute of Chemical Physics, Russian Academy of Sciences, CARTER WHITE, Naval Research Laboratory — Understanding of initiation chemistry of shock-compressed energetic materials on the atomic scale is one of the outstanding problems for shock wave and energetic materials community. Using first-principles density functional theory, we have performed molecular dynamics simulations of the reactive molecular collisions of several energetic molecules such as PETN and RDX aimed at elucidating the first chemical events that trigger the chemistry behind the shock wave front. These results provide an insight into fundamental mechanisms responsible for the transformation of mechanical energy from the shock wave into molecular degrees of freedom that result in excitation of a reaction mode, bond breaking and subsequent events taking place under non-equilibrium conditions of the shock wave environment.
8:45AM U2.00004 Theoretical studies of shock-induced plastic deformation and phase transformations in RDX

MARCEWELL, THOMAS SEWELL, Theoretical Division, Los Alamos National Laboratory — The relationships between shock-induced plastic deformation and initiation sensitivity have been studied in RDX using MD simulations. Homogeneous defect nucleation in (100), (111) and (210) oriented single crystals has been studied under shock loading at particle velocities of 420, 630 and 840 m/s. Deformation by shear-bands was seen in shocks parallel to [100] at particle velocities ≥ 630 m/s. No evidence was found for homogeneous nucleation of defects such as dislocations or shear-bands in shocks normal to (111) and (210) at particle velocity. These results are consistent with the steric hindrance model for initiation sensitivity and flyer plate studies of oriented RDX single crystals. The collapse of 20 nm diameter cylindrical voids was studied under the same conditions mentioned above. A variety of anisotropic material responses occur, along with significant increases in intramolecular temperatures, as the voids collapsed. Also, a previously unknown shock-induced phase transformation was observed during shocks normal to (210). This phase transformation occurs homogeneously for shocks parallel to [010] at particle velocities greater than 1 km/s. The Hugoniot for shock loading in this direction has been calculated for a defect free crystal, allowing for direct experimental assessment of this prediction. LA-UR-07-1016

9:00AM U2.00005 A semi-metallic layer in detonating nitromethane

KURT GLAESEMANN, Lawrence Livermore National Laboratory, JOHN JOANNOPoulos, Massachusetts Institute of Technology — We present the first ever glimpse behind a detonation front in a chemically reactive quantum molecular dynamics simulation (up to 0.2 ns) of the explosive nitromethane (CH₃NO₂), represented by the density-functional-based tight-binding method (DFTB). This simulation is enabled by our recently developed multi-scale shock wave molecular dynamics technique (MSST) that opens the door to longer duration simulations by several orders of magnitude. The electronic DOS an important role in the density of states evolution and a possible Mott metal-insulator transition. This work was performed under the auspices of the US Department of Energy by the University of California, LLNL under contract number W-7405-Eng-48.

9:15AM U2.00006 Atomic Simulations of Detonation Instabilities in Condensed Phase Systems

EDWARD KOBER, ANDREW HEIM, TIMOTHY GERMANN, LANL, NIELS JENSEN, UC Davis — We report the results of simulations of condensed phase detonation phenomena using a model diatomic system: 2AB -> A₂ + B₂. The initial set of parameters for this system corresponded to the Model 0 set of C. White et al, which exhibits a steady, Chapman-Jouget (CJ) detonation structure with a reaction zone length of 30-100 Å. This has a highly compressed CJ state (V/V₀ ~0.5) that does not consist of discrete molecular species. The potential form was modified so that a more molecular CJ state resulted, consistent with the models for conventional organic explosives. The new system has a less dense CJ state (V/V₀ ~0.8), and the reaction zone was substantially extended. The reaction rate fits Arrhenius-type kinetics with an activation energy of ~2 eV, with a minor density dependence. In contrast, the original Model 0 system had a lower activation energy (~1 eV) with a stronger density dependence. The new system exhibits quite marked two dimensional instability structures with well-defined wavelengths similar to what has been observed for gas-phase detonations and for nitromethane. Depending on the exothermicity and the width of the periodic simulations, instabilities can result in either detonation failure or quasi-steady propagation. The observed instability velocities are several per cent higher than CJ values derived from thermodynamic analyses.

Friday, June 29, 2007 8:00AM - 10:00AM —
Session U3 Phase Transitions IV
Fairmont Orchid Hotel Plaza I

8:00AM U3.00001 Response of silicon to shock wave compression along [100] and [111] orientations

STEVEN J. TURNBAUSE, Y.M. GUPTA, Washington State University — Silicon is a high strength, brittle solid that undergoes multiple compression induced phase transformations. To complement x-ray diffraction measurements to examine inelastic deformation and phase transformations in shocked Si, we have examined the continuum response of silicon under shock compression. Transmitted wave profiles were measured at Si/LiF interfaces using a velocity interferometer. Peak stresses ranged between 11 and 22 GPa. The measured HELs were 9.2 GPa and 7.7 GPa for [100] and [111] orientations, respectively. Following the phase transformation, which occurred at about 13.5GPa, the volume compression was roughly 23% for peak stresses ranging from 15 to 22 GPa. This volume compression is consistent with a completed phase transformation and is much larger than previously reported volume compressions [1,2]. Work supported by DOE. [1] W. H. Gust and E. B. Royce, J. Appl. Phys. 42, 1897 (1971). [2] T. Goto et al., Jap. J. Appl. Phys. 21, L369 (1982).

8:15AM U3.00002 Dynamic response of pure titanium up to 1300 K

EUGENE ZARETSKSY, Ben-Gurion University — Dynamic response (yield and strength) of pure polycrystalline Ti (Alfa Aesar, 99.99% Ti) was studied in a series of planar impact experiments with initial sample temperature ranged from 300 to 1300 K. In the separate series of experiments the temperature dependence of the longitudinal speed of sound in Ti was measured on the base of the reverberation of the stress pulse generated in the 3-mm Ti sample by 1-mm aluminum impactor. In all the experiments the velocity of the sample free surface was continuously monitored by VISAR. It was found that in spite of a softening preceding the HCP-BCC transformation in titanium (1155 K) the HCP phase stays upon the HCP-BCC transformation, which occurs at about 13.5GPa, approximately 23% for peak stress ranging from 15 to 22 GPa. This volume compression is consistent with a completed phase transformation and is much larger than previously reported volume compressions. In all the experiments the strength mechanisms caused by the temperature increase and the phase transition are discussed.

8:30AM U3.00003 Structural and Chemical Changes in Pyrene Crystals under Static High Pressures

BAOZHOU SUN, ZBIGNIEW DREGER, YOGENDRA GUPTA, Washington State University — To gain insight into the response of molecular crystals to high pressures, pyrene crystals were examined in diamond-anvil cell experiments using Raman and FTIR spectroscopy. Three distinct Raman spectra were observed around 0.5 GPa, depending on the type of pressure transmitting medium. It was demonstrated that pyrene I: (i) transforms to pyrene II, in water and mineral oil, (ii) transforms to pyrene III, in argon and nitrogen and (iii) remains in the same phase, in solid media. These changes are discussed in terms of nonhydrostatic pressure transmitting media and intercalation of medium and sample. Irreversible chemical changes were observed upon compressing pyrene above 25 and 40 GPa. Recovered product was examined using FTIR spectroscopy indicating gradual transformation to an amorphous hydrogenated carbon structure. Work supported by DOE and ONR.
8:45AM U3.00004 Initial Temperature Effects on the Dielectric Properties of PZT 95/5 During Shock Compression

A strong electric field is generated when the shock-induced depoling current from a normally poled PZT 95/5 sample is passed through a large resistive load. The portion of total depoling current that is retained on the sample electrodes to account for capacitance is governed by the dynamic dielectric properties of both unshocked and shocked PZT 95/5. Early studies used measured load currents from single samples to assess models for dielectric response. More recent studies used shock-driven circuits in which multiple PZT 95/5 elements were displaced both parallel and perpendicular to the shock motion. This allowed both load and charging currents to be measured for individual elements that are subjected to shock compression and release at different times. In the present study, these techniques have been utilized to examine dielectric properties in PZT 95/5 samples at initial temperatures from -50 to 70 °C. Measured currents show large temperature effects on dielectric properties, and different models for dielectric response have been examined for simulating these results.

9:00AM U3.00005 Study of near critical point states of tantalum and lithium by pulse heating under launching

— VLADIMIR TERNVOIT, DMITRY NIKOLAEV, SERGEY KVITOV, ALEXEY PYALLING, VLADIMIR FORTOW, IPCP RAS

— The near critical point states of the liquid–vapor phase transition of tantalum and lithium were investigated. The heating of tantalum foil samples in 1-D geometry was carried out by multiple-shocked He from back side of the tantalum foil and heating of lithium - by shocked He from the front side under dynamically created isobaric conditions. The temperature of sample was measured by fast 6-channel optical pyrometer. The energy was obtained from measured shock velocity in He using stepped transparent window. Two sets of experiments with various history of heating were carried out, allowed to evaluate the critical point location of the studied metals in P-T plane.

9:15AM U3.00006 Simulation of phase transitions and material decomposition in ultrashort laser–metal interaction

MIKHAIL POVRANTSHYN, PAVEL LEVASHOV, KONSTANTIN KHISHCHENKO, Institute for High Energy Densities, JIHT RAS

— A numerical hydrodynamic study of femtosecond laser irradiation (800 nm, 100 fs, 10^{12}–5×10^{13} W/cm^2) of metal targets (Al, Au, Cu) is presented. A detailed analysis of laser induced phase transitions, melting wave propagation and material decomposition is performed using a thermodynamically complete two-temperature equation of state with separate stable and metastable phase states and phase boundaries. Material evaporation from the target surface and fast melting wave propagation into the bulk are observed. Investigation of the phase trajectories of different target layers shows the presence of the metastable states in rarefaction wave. The lifetime of the metastable liquid state is estimated by means of the theory of homogeneous nucleation. Mechanical fragmentation of the target material at high strain rates is controlled with the help of Grady criterion. As a result, several ablation mechanisms are observed. A major fraction of the ablated material, however, is found to originate from the metastable liquid region, which is decomposed either thermally at the vicinity of the critical point into a liquid–gas mixture, or mechanically at high strain rate and negative pressure into liquid droplets and chunks. The calculation results explain available experimental findings.

9:30AM U3.00007 Study of Phase Transitions in Cerium by Pressure Gauge PVDF

MIKHAIL ZHERNOKLETOV, VLADIMIR SIMAKOV, VALERY BORISSENOK, VIACHESLAV BRAGUNETS, VASYLIO VOLGIN, RFNC-VNIIEF, FRANK CHERNIE, MARVIN ZOCHER, LANL, RFNC-VNIIEF TEAM, LANL TEAM

This paper examines phase transitions in cerium during shock compression using PVDF gauges. A two-wave structure was observed with loading pressures of 4GPa - 12GPa. The wave structure consists of leading isentropic compression wave followed by a shock wave. This wave structure was formed as a result of the isomorphic (γ − α) phase transition. The wave profiles exhibited no peculiarities resulting from the polymorphic transition (α − ε) as predicted by Elkin et al [Proceedings of the International Conference VII Kharton Readings, Sarov 2005, p. 116].

9:45AM U3.00008 Measurement of sound velocities and shear strength of cerium under shock compression

ALEXEI KOVALEV, MIKHAIL ZHERNOKLETOV, VLADIMIR KOMISSAROV, MIKHAIL NOVIKOV, RFNC-VNIIEF TEAM

Sound velocity in shock-compressed cerium was measured in the pressure range of 35−140GPa by the rarefaction overtake technique with use of the indicator liquids carbogal and tetrachloromethane. The samples were loaded by generators of planar shock waves based on use of powerful HE. Luminescence of the liquid indicators was recorded by optical gauges based on photodiode FD256. In the pressure range of 13−35GPa, sound velocity was measured in cerium samples by the method of counter release with use of manganin-based piezoresistive gauges. Initial density of cerium samples was 6.75g/cub.cm. Basing on the measured values of longitudinal and volume sound velocities, Poisson ratio and shear strength of cerium were determined, boundaries of melting at shock adiabat were revealed. Experimental data were compared to calculation results.

Friday, June 29, 2007 8:00AM - 9:30AM – Session U4 Inelastic Deformation V

Fairmont Orchid Hotel Plaza II

8:00AM U4.00001 Transformation of voids observed on a surface to a volumetric size distribution

LYNN SEAMAN, SRI International — A new procedure, based on the Scheil method, for transforming surface counts of voids or grains to volumetric size distributions has been developed. The method simultaneously smooths the surface count data and produces the volumetric distribution. A constraint has been added to require that the relative volume of the voids or grains matches the relative area of these artifacts. Here the method is applied to void count data from small experiments in 99.999% pure aluminum performed by Qi MeiLan and similar experiments in several other materials.


2 Qi MeiLan, PhD thesis, to be published.
Simulation results are consistent very well with the experimental results. The spherical projectile materials are aluminum, steel and copper. All bumper materials are aluminum alloy 6061-T6. The simulation velocities were in the different combination of impact velocities and bumper-thicker-to-projectile-diameter ratios (t/D) has been performed using the SPH technique of AUTODYN. The numerical simulation of fragmentation onset velocity of different material projectile hypervelocity impacts on bumpers with fragmentation onset velocity. To determine the fragmentation onset velocity experimentally, a number of experiments have been conducted with different projectile/bumper configuration. The numerical simulation of fragmentation onset velocity of different material projectile hypervelocity impacts on bumpers with different combination of impact velocities and bumper-thicker-to-projectile-diameter ratios (t/D) has been performed using the SPH technique of AUTODYN. The spherical projectile materials are aluminum, steel and copper. All bumper materials are aluminum alloy 6061-T6. The simulation velocities were in the range of 1km/s-7km/s. The ratios of t/D were varied from 0.01 to 0.80. The material models were consisted of Mie-Gruniesen (shock) equation of state, Steinberg-Guinan strength model and Grady fragmentation failure model. The simulation results are given and compared with the experimental results. The simulation results are consistent very well with the experimental results.

Numerical Simulations of Fragmentation Onset Velocity of Projectile Impact on Thin Bumper. WEI ZHANG, Harbin Institute of Technology, CAIXIA JIANG, WENLAI MA, BAOJUN PANG, HYPERVERCLOCITY IMPACT RESEARCH CENTER TEAM — The conventional spacecraft meteoroids and orbital debris shielding system is the Whipple shield. In general there is a threshold velocity that is just sufficient to shatter the projectile for each system consisting of a projectile and bumper. This velocity is known as the fragmentation onset velocity. To determine the fragmentation onset velocity experimentally, a number of experiments have been conducted with different projectile/bumper configuration. The numerical simulation of fragmentation onset velocity of different material projectile hypervelocity impacts on bumpers with different combination of impact velocities and bumper-thicker-to-projectile-diameter ratios (t/D) has been performed using the SPH technique of AUTODYN. The spherical projectile materials are aluminum, steel and copper. All bumper materials are aluminum alloy 6061-T6. The simulation velocities were in the range of 1km/s-7km/s. The ratios of t/D were varied from 0.01 to 0.80. The material models were consisted of Mie-Gruniesen (shock) equation of state, Steinberg-Guinan strength model and Grady fragmentation failure model. The simulation results are given and compared with the experimental results. The simulation results are consistent very well with the experimental results.

Studies on the Fracture of HR-2 Steel Cylinder under Implosion. HAIBO HU, TIEGANG TANG, QINGZHONG LI, XUELING SUN — The fracture phenomena of HR-2 steel cylinder under implosion loading are studied by the dynamic technologies of X-flash photography and high-speed photography. The results of X-flash photography show that the thermo-plastic instability and fracture have occurred in the HR-2 steel cylinder wall during the implosion loading process. The initiation and propagation processes of cracks on the inner wall of the hemi-cylinder have been directly observed by the high-speed photography. The comparison between the two kinds of experimental results shows that the cracks initiate firstly in the inner wall of the steel cylinder. There are clear shear characteristics on the collected fragments. The metallography examinations show that the adiabatic shear bands and microcracks initiate first near the inner wall of the steel cylinder, and propagate along the maximum shear stress paths, which agrees with the previous deduction of experiments. With loading pressure increasing, the dimension of fragments and the width of ABS both become smaller.

Longitudinal Fracture Propagation of Explosive Loaded Metal Shells. HAIBO HU, TIEGANG TANG, BAYI HU, Institute of Fluid Physics, CAEP — Longitudinal fracture propagation behavior in self-organized shear bands is discussed. Shear fracture can propagate longitudinally tens of mm, while recovery observations show that fracture surface is consisted of shear fracture cells in mm length. They locate approximately along a given generatrix and coalesce longitudinally at some stage of growth breaking through shell wall. Analysis on alignment phenomenon of shear initiations, considering up-stream shear initiations influence, is given. Early shear initiations can influence sites of shear instability on neighboring down-stream section by changing local stress field within a time gap sufficient for mechanical wave propagation. It leads to shear initiation in given orientation and location along given generatrix in competition with random shear initiations. Knowing conditions for such mechanism keep on work layer after layers, not to be broken, is of importance. Simulate multi shears coalesce using a mono fracture growth model is not advisable, while to simulate the growth of tongue like shear bands individually, calculating instantaneous stress field in 3D space is a tremendous work. To approximate such kind of process for credible modeling is important. For fragment size distribution predication, in well known models there is not adequate consideration of longitudinal propagation factor, which depends on material parameters and loading conditions.

The Puzzle of Explosive Response to Shock: Complexity to Simplicity by Changing the Observational Scale. HUGH JAMES, AWE, Aldermaston — At the mesoscale the shock interaction with a heterogeneous explosive is a complex mix of wave interactions with density discontinuities, localized heating, transient chemical reactions and multiphase flows. However, the macroscopic response can often be described in terms of simple phenomenological models. Those describing initiation thresholds and the onset of detonation have long been known and are widely used. This paper shows that simplicity at the continuum level is observed over a much larger range of explosive responses; from the parallel behaviours of the different markers present during reaction growth, to the simple rules for scaling in-material gauge results. The transition from complex trigger to simple response currently provides one of the great challenges for understanding explosive behaviour, and aspects of this transition will be explored and discussed.
8:30AM U6.00002 Effect of Transverse Electric Field on Sensitivity of an 88% by Weight HMX Based Energetic Material, RICHARD LEE, JERRY FORBES, NSWC Indian Head, EDWARD PALERMO, University of Michigan, WILLIAM WILSON, DTRA — Thresholds for shock sensitivity were determined for explosive samples with and without applied fields using a variation of the Navy’s modified gap test. Rectangular charges (76 mm wide x 12.7 mm long x 5 mm thick) confined on two sides by 50.8 mm thick bars of Teflon were shock loaded using the Navy’s standard large scale gap test donor system. Free surface velocity at the opposite end of the sample (12.7 mm from input surface) was measured using a high-speed camera. Velocity versus input pressure plots highlight thresholds for first reaction, deflagration, and detonation. In addition the use of an intensified high-speed electronic camera provided a clear differentiation of when the products were self-luminous, directly confirming initiation. Electric fields were applied transverse to the shock direction via thin foil electrodes. These electrodes were held in place by the Teflon insulation. The data shows that this energetic material requires less input pressure to ignite the reaction with voltages of 5 kV applied across the 5 mm thick sample as compared to results without a field.

8:45AM U6.00003 Shock Initiation Thresholds for Insensitive High Explosives, HUGH JAMES, AWE — Work with conventional high explosives shows that the initiation thresholds for a variety of projectile types can be mapped onto a single curve in a space defined by the pressure or particle velocity of the initial shock, and the time of the maximum non-divergent shock volume generated in the explosive by the initial impact. This curve is distinct from that observed for high explosives, where maximum reaction growth occurs at the time of detonation. In contrast for an insensitive high explosive, the location of the initiation thresholds in the above space appear divided between those forming a distinct threshold curve and those which appear to be a continuation of the Pop Plot. Projectile diameters larger than the failure diameter still form a distinct threshold, but smaller projectile diameters lie on the Pop Plot curve. An examination of the data indicates that impacts lying on the threshold curve produce non-divergent detonations. These detonations appear likely to remain non-divergent or even fade. The initial conditions need to be enhanced so that the impact lies on, or just above, the Pop Plot before divergence takes place. Those initial conditions that lie on the Pop Plot only need sufficient run distance in the explosive before a diverging detonation is achieved.

9:00AM U6.00004 A Study of SDT in an Ammonium Nitrate (NH₄NO₃) Based Granular Explosive, MALCOLM BURNS, PETER TAYLOR, AWE — In order to study the SDT process in a granular non ideal explosive (NIE) an experimental technique has been developed that allows the granular explosive to be shock initiated at a well controlled “tap density”. The granular NIE was contained in a PMMA cone and a planar shock was delivered to the explosive through buffer plates of varying material. A combination of piezoelectric probes, ionization pins, PVDF stress gauges and a high speed framing camera were used to measure the input shock pressure and shock and detonation wave positions in the explosive. Four trials were performed to characterize the run to detonation distance versus pressure relationship (Pop plot) of the granular NH₄NO₃ explosive. Input pressures ranged from close to the 4GPa predicted CJ pressure of the granular explosive down to 1.4 GPa, giving run distances up to 14mm for the lowest pressure. The data indicates a steady acceleration of the input shock to the detonation velocity, implying significant reaction growth at the shock front. This is in contrast to the behaviour of most high density pressed PBXs which show little growth in shock front velocity before transit to detonation. The experimentally observed initiation behaviour is compared to that predicted by a simple JWL++ reactive burn model for the granular NH₄NO₃ explosive which has been fitted to other detonics experiments on this material.

9:15AM U6.00005 Shock Reactivity Study on Standard and Reduced Sensitivity RDX of Different Particle Size Distributions, NICHOLAS MCGREGOR, Naval Surface Warfare Center, Indian Head Division, ALLEN LINDFORS, Naval Air Warfare Center, and MALCOLM BURNS, AWE. Four monomodal experimental compositions containing 73% solids by weight and 27% HTPB binder were tested. The compositions were made using either standard or reduced sensitivity grades of RDX in Class 5 or Class 1 150-300 micron sieve cut particle size classes. Results have shown marked changes in the mode of reaction between the two particle size classes. Both RDX grades at the Class 1 sieve cut particle size distribution showed significant reaction at the shock front as well as behind the front. The Class 5 RDX compositions however showed little reaction at the shock front with rapid growth behind the front. Similar input pressures resulted in a full detonation in a similar distance for like RDX grades. Reaction modes were similar but occurring at greater input pressures for the reduced sensitivity grade of RDX compared to the corresponding particle size distribution standard grade RDX counterpart.

9:30AM U6.00006 Initiation of Explosives From the Bow Shock of a Supersonic Penetrator, ERIC N. FERM1 Los Alamos National Laboratory — An analytic and computational study of supersonic penetration of an explosive is presented. The goal is the development of an initiation criterion relating projectile diameter and threshold projectile velocity determined by fundamental material and explosive parameters. The basis of the initiation criterion is an examination of the steady flow structure around a supersonic penetrator in the unreacted materials, yielding the states along the bow shock and the size and sonic character of the flow structure. The state is used to determine the time scale of the reacting explosive using initiation experiment results (Pop Plot). The size of the subsonic region is compared to the failure diameter to examine the viability of the initiation. The results are compared with experimental initiation criterion.

1 LA-UR-07-1046

9:45AM U6.00007 Coherence for the Critical Condition of DDT and SDT in Energetic Materials, HUAN SHI, TAN XIANQIANG, Guangzhou University — Most of the past research for the energetic materials focused on the SDT for explosives and DDT for solid propellants. Since the difference between the explosive and solid propellant decreases with the increase of the energy density in the solid propellant, the study of SDT for the solid propellant is needed. In this paper, two-dimensional SDT experiments and thin wall copper DDT experiments have been carried out for two types explosives[E1(95% RDX), E2(95% HMX)] and two types solid propellants[P1(55% RDX), P2(55% HMX)] to investigate the coherency for the critical conditions of SDT and DDT for the same energetic materials. The results show that E1 has the highest sensitivity in both the SDT and DDT tests followed by E2, P1 and P2. Although such rules cannot be generalized to all high energetic materials, it is obvious that a relationship exists between SDT and DDT sensitivity. The relationship between the deflagration hazard in SDT and the combustion hazard in DDT is critical in this study. The measured critical conditions and parameters such as the increase velocity of combustion peak, the highest scope and the movement velocity in SDT indicated that coherency exists between the SDT and DDT.

1 Sponsored by the National Science Foundation of China -NSAF (10276015)

Friday, June 29, 2007 10:30AM - 12:30PM — Session V2 Continuum and Multiscale Modeling III Fairmont Orchid Hotel Amphitheater
10:30AM V2.00001 Void Growth and Coalescence Nanocrystalline Metals: Molecular Dynamics Modeling, Continuum Modeling, and Experiments. DAVID BENSON, SIRIRAT TRAIVIRATANA, MARC MEYERS, PARAG DIXIT, UCSD, ALICE KONGES, DAN KALANTAR, LLNL. Fragmentation of the support structures in ICF experiments, leading to the damage of instrumentation and optics, is currently a concern as new research facilities are brought on line. The current research focuses on understanding the void formation and growth mechanisms. MD simulations in single and polycrystalline nano-materials have been carried out with LAMMPS. Void growth occurred by the emission of shear dislocation loops. Continuum finite difference calculations of the same Voronoi-generated microstructure were also performed using ALE-AMR. The results of the calculations are compared to each other and to laser shock experiments in thin vanadium films. This research was supported by LLNL grant B585558.

10:45AM V2.00002 Numerical simulation of interaction of hypervelocity particle stream with a target. ILYA LOMOV, BENJAMIN LIU, VLAD GEORGEVICH, TARABAY ANTOUN, LLNL. The Distinct Element Method (DEM) is one of the particle methods and is generally applied to granular materials and particle target material properties and surrounding air properties. We ran 3D calibration simulations with up to 10 million individual particles and conducted sensitivity studies with 2D cylindrically symmetric simulations. We used an Eulerian Godunov hydrocode with adaptive mesh refinement. The particles, target material and air are represented with volume-of-fluid approach. Brittle particle and target material has been simulated with pressure-dependent yield strength and Steinberg model has been used for metal targets. Simulations demonstrated penetration depth and a hole diameter similar to experimental observations and can explain the influence of parameters of the stream on the character of the penetration.


11:15AM V2.00004 Simulation of Comet Impact and Survivability of Organic Compounds. BENJAMIN LIU, ILYA LOMOV, LLNL, JENNIFER BLANK, SETI Institute, TARABAY ANTOUN, LLNL. Comets have been proposed as a mechanism for the transport of complex organic compounds to Earth. For this to occur, a significant fraction of organic compounds must survive the shock loading, in particular the high temperatures, due to impact. 2D and 3D numerical simulations were performed to study the thermodynamic states due to a comet impact. The comet was modeled as a 1-km diameter icy sphere traveling at the Earth’s escape velocity (11 km/s) impacting a half-space of basalt. Simulations were performed with GEODYN, a parallel, multi-material, Godunov-based Eulerian code employing adaptive mesh refinement. A constitutive model calibrated for hard rock was used for basalt. Tabular equations of state were used to account for the extreme conditions present upon shock loading. A major focus of the study was tracking the thermodynamic state of the comet material. Both the maximum temperature experienced and the phase were tracked for each point in the comet. Temperature histories in the comet were also recorded. These quantities were used to estimate viability of organic compounds upon impact. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

11:30AM V2.00005 Implementation of the TEPLA Damage Model in a 3D Eulerian Hydrocode. KATHLEEN S. HOLIAN, SEAN P. CLANCY, PAUL J. MAUDLIN, Los Alamos National Laboratory. A sophisticated damage model (TEPLA) has been implemented into a three-dimensional (Cartesian) computer code (Pagosa) used here at Los Alamos National Laboratory. TEPLA was originally an isotropic damage model based upon the Gurson flow surface (a potential function used in conjunction with the associated flow law) that models damage due to both porosity growth and plastic strain. It has since been modified to model anisotropic elastoplastic material strength as well. Pagosa is an Eulerian hydrodynamics code that has the following special features: a predictor-corrector Lagrangian step that advances the state variables in time, a high-order advection algorithm that remaps the problem back to the original mesh every time step, and a material interface tracking scheme with van Leer monotonic advection. It also includes a variety of equation of state, strength, fracture, and high explosive burn models. We will describe the physics of the TEPLA model (that models both strength and damage) and will show preliminary results of test problems that are used to validate the model. The four test problems (simple shear, stretching rod, Taylor anvil, and plate impact) can be compared with either analytic solutions or with experimental data.

11:45AM V2.00006 Numerical Simulation of high velocity impact phenomenon by the Distinct Element Method (DEM). YOKO TSUKAHARA, AKIKO MATSUO, Keio University, KATSUMI TANAKA, National Institute of Advanced Industrial Science and Technology. The Distinct Element Method (DEM) is one of the particle methods and is generally applied to granular materials and incompressible elastic materials. DEM with elastic-plastic deformation is developed for simulations of shock loading phenomenon in condensed media, and is applied to problems with large deformations. DEM gives more stable results than Lagrangian Finite Difference or Finite Element Method. Numerical oscillations are reduced by the consideration of artificial viscosity. The hydrodynamic constitutive law is introduced to the DEM, and the dynamic behaviors of materials, such as metals and concretes, under high velocity impact phenomenon are well compared with experimental and other computational results.

12:00PM V2.00007 Numerical Studies on the Explosive Welding by Smoothed Particle Hydrodynamics (SPH). KATSUMI TANAKA, National Institute of Advanced Industrial Science and Technology. A particular characteristic of an explosively produced weld is that the profile of the weld interface often has a regular wavy appearance. An effect of detached shock wave and jetting on the metal interface of explosive welding has been shown by SPH (Smoothed particle hydrodynamics). Numerical results show wavy interface which is observed in several experiments. High speed jet between interface and Karman vortex after oblique impact of a flyer plate to a parent plate were major mechanism of explosive welding.
12:15PM V2.00008 Structural-Scaling Transitions in Microshear Ensembles and Self-Similarity of Wave Fronts and Failure in Shocked Materials
OLEG NAIMARK, Institute of Continuous Media Mechanics of RAS — Statistical theory of mesoeffects allowed establishment of new type of critical phenomena—structural-scaling transitions, to develop thermodynamics and phenomenology in terms of defect density tensor and structural scaling parameter, which reflects scaling transition and generation of collective modes of defects: shear transformation zones (STZ) and damage transformation zone (DTZ), which provide plastic relaxation and damage-failure transition. Shock wave experiments and structural study supported linkage of these modes with material responses in large range of load intensity and allowed interpretation: (i) mechanisms of failure wave generation and propagation that has the nature of delayed failure needed for excitation time of blow-up collective modes. Experimental study of failure wave generation and propagation was analyzed for Taylor test in fused quartz rod using high-speed framing and supported "delayed" mechanism of failure wave generation; (ii) self-similarity of wave fronts under reloading and unloading, fourth power universality of steady-state plastic was confirmed both theoretically and experimentally in plate impact test for copper and using NEW VIEW scaling analysis of STZ distribution in recovered specimen; (ii) transition from thermo-activation kinetics of plastic relaxation to steady-state relaxation and overdriven shock regime.

Friday, June 29, 2007 10:30AM - 12:30PM
Session V4 Inelastic Deformation VI
Fairmont Orchid Hotel Plaza II

10:30AM V4.00001 Statistics of Spall and Hugoniot Elastic Limit from Line VISAR
MICHAEL FURNISH, TRACY VOGLER, C. SCOTT ALEXANDER, WILLIAM REINHART, WAYNE TROTT, LALIT CHHABILDAS, Sandia National Laboratories — Material heterogeneity appears to give rise to variability in the yield behavior of ceramics and metals under shock loading and spall conditions. The line-imaging VISAR provides a way to measure this variability, which may then be quantified by Weibull statistics or other methods. Weibull methods assign a 2-parameter representation of failure phenomena and variability. We have conducted experiments with tantalu (25 and 40 um grains), soda lime glass, single-crystal sapphire and silicon carbide. Line-imaging VISAR data reveal an averaged velocity response analogous to point VISAR or PDV data. As well, in addition to strength variability information, this diagnostic provides statistical bounds for the velocity histories, measurements of surface distortion with time (length scales and amplitudes), and verification of sample edge effects and wave focusing. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

10:45AM V4.00002 Hydrocode modeling and an experimental study of explosively driven water jets
PHILIP RAE, PETER DICKSON, ALAN NOVAK, GARY PARKER, Los Alamos National Laboratory — There is currently interest in water based penetrators. The research to be presented is an experimental and numerical study of the generation of fast (> 4 - 5 km s \(^{-1}\)) jets of water from a charged shape like device. High-speed and Schlieren photography techniques have been used to record the jets produced by various design iterations and the experimental images compared to models run in the CTH hydrocode. The computer code was used to reduce the number of experiments required to solve some initial problems with non-uniform initial jet shapes. The CTH code has been successful in modeling the observed jets, but only after careful attention was paid to the equation-of-state used for the water. Initially the jet diameter produced by the code was considerably thinner than experimentally observed. A much better match occurred when the most modern SESAME EOS table for water was used.

11:00AM V4.00003 Study of the projectile impact on aluminum targets divided by water
TEI SABURI, SHIRO KUBOTA, YUJI OGATA, YUJI WADA, National Institute of Advanced Industrial Science and Technology, TOSHIKAZU NAKANISHI, KOMATSU Ltd. — The impact behavior of a projectile into aluminum alloy targets divided by water was experimentally observed using high-speed video camera, and a numerical simulation was conducted using LS-DYNA. The target size was 5mm in thick, 200mm in height and width. Two target plates were positioned parallel at a distance of 120-180mm, and the space between targets was filled up with water. A SNMC steel projectile was 10mm in height, and 10mm in diameter. The projectile was accelerated by a compact accelerator using an explosive, and impacted on the first target. Impact experiments without water in the gap space were also conducted. In case without water, the projectile penetrated both two targets. On the other hand, in case that water fills up in the gap, The projectile did not penetrate the second target plate, and the both target plates were entirely and largely deformed compared with the case that water is absent. Numerical simulation of the projectile impact was conducted using a finite element code of LS-DYNA. ALE(Arbitrary Lagrangian Eulerian) method was adopted to simulate fluid-structure interaction problem. The deformation behavior of targets was confirmed by the simulation, and the importance of water effect on the deformation of the targets and the de-acceleration of the projectile velocity was shown.

11:15AM V4.00004 Damaging of materials by bi-dimensional dynamic effects
M. BOUSTIE, J.P. CUQLELANDAIS, L. BERTHE, CNRS, S. BARRADAS, ENSMP, LCD, PHILIPPE BASTIEN, C. BOLIS, M. ARRIGONI, T. DE RESSEGUIER, CNRS, M. JEANDIN, ENSMP, LCD, MARTIN COMPANY, INC. — The impact behavior of a projectile into aluminum alloy targets divided by water was experimentally observed using high-speed video camera, and a numerical simulation was conducted using LS-DYNA. The target size was 5mm in thick, 200mm in height and width. Two target plates were positioned parallel at a distance of 120-180mm, and the space between targets was filled up with water. A SNMC steel projectile was 10mm in height, and 10mm in diameter. The projectile was accelerated by a compact accelerator using an explosive, and impacted on the first target. Impact experiments without water in the gap space were also conducted. In case without water, the projectile penetrated both two targets. On the other hand, in case that water fills up in the gap, The projectile did not penetrate the second target plate, and the both target plates were entirely and largely deformed compared with the case that water is absent. Numerical simulation of the projectile impact was conducted using a finite element code of LS-DYNA. ALE(Arbitrary Lagrangian Eulerian) method was adopted to simulate fluid-structure interaction problem. The deformation behavior of targets was confirmed by the simulation, and the importance of water effect on the deformation of the targets and the de-acceleration of the projectile velocity was shown.

11:30AM V4.00005 Examination of the spallation behavior of cerium metal, FRANK CHERNE, PAULO RIGG, WILLIAM ANDERSON, JASON COOLEY, Los Alamos National Laboratory — We have conducted a series of free surface shock experiments on cerium metal at peak shock pressures from 0.9-7.6 GPa. These experiments were done to examine the elastic-plastic behavior, the solid-liquid phase transition occurring at 0.7-0.8 GPa, and the spall strength of the material as a function of peak stress. The elastic and low-pressure plastic waves exhibit long rise times, while the post-formation plastic wave is sharp. Spallation profiles obtained from using optical techniques will be presented and discussed.

11:45AM V4.00006 Ductile spall in copper of different structure
B. HERRMANN, E. ZARETSKY, Ben Gurion University, Beer Sheva, Israel; G.I. KANEL, Joint Institute for High Temperatures, Moscow, Russia, S.V. RAZORENOV, Institute of Problems of Chemical Physics, Chernogolovka, Russia — The spall signals and post mortem metallurgy of crystals of Cu+0.1%Si solid solution and copper with sub-micron silica inclusions were studied in planar impact experiments at two different load durations. The samples contained large (4-5 mm in diameter) grains with 1000 µm diameter. The fracture surfaces of copper with silica inclusions are covered by a net of dimples of 1 µm to 50 µm diameter. The fracture of the spall surfaces correlate with the free surface velocity histories. The main fracture surface of the Cu+0.1%Si grains consists of dimples ~5 µm to 50 µm diameter. The fracture surfaces of copper with silica inclusions are covered by a net of dimples of 1 µm to 5 µm diameter. The free surface velocity histories demonstrate prolonged spall fracture process for Cu+0.1%Si samples and faster fracture at lower fracture stress for copper with brittle inclusions.

1Supported by the US DOE under contract DE-AC52-06NA25396.
12:00PM V4.00007 Crack-resistance and spall strength of cerium under dynamic loading. VICTOR PUSHKOV, VLADIMIR OGORODNIKOV, SERGEY ERUNOV, Russian Federal Nuclear Center-VNIIEF — There is poor knowledge on cerium characteristics under dynamic loading, such as dynamic crack-resistance and spall strength, which are important for some applications. For example, material crack-resistance is one of parameters of the model, which is used for numerical description of the dispersion process [1]. Tests were performed for determination of dynamic crack-resistance by the split Hopkinson pressure bar method. However, significant plasticity of cerium caused failure of crack-resistance determination. Therefore crack-resistance evaluation was performed by study of material spall strength $\sigma_0$. Considering value $\sigma_0$, it is possible to determine specific work for material break $\Psi$ [2], and, basing on it, then it is possible to determine crack-resistance value by the Irvine-Griffiths criterion. 


12:15PM V4.00008 Instability of an Interface Between Steel layers Acted Upon by an Oblique Shock Wave. OLEG DRENNOV, RFNC-VNIIEF — The results of experiments in which development of instability was observed on the interface between two identical metals in tight contact with passage of an oblique shock wave through it are presented. The loading scheme is shown in figure 1. The photograph of microsection of the contact boundary after shock-wave loading is shown in figure 2.

The calculations showed that perturbations develop only in the presence of a technological microgap of several micrometers between the metal layers. Unloading of the material behind the oblique shock front into the gap gives rise to considerable short term velocity gradient $t < 0.2 \mu s; \Delta U > 3 \mu m/\mu s$. Simultaneously, near the interface behind the wave front there is a short-term loss of strength of the material due to thermal softening and the heterogeneous nature of the deformation.

Friday, June 29, 2007 10:30AM - 12:15PM –
Session V6 Explosives Thermal/Mechanical Response Fairmont Orchid Hotel Promenade I/II

10:30AM V6.00001 Violent Reactions from Non-Shock Stimuli. HAROLD SANDUSKY, NAVSEA Indian Head Division — Most reactions are thermally initiated, whether from direct heating or dissipation of energy from mechanical, shock, or electrical stimuli. For other than prompt shock initiation, the reaction must be able to spread through porosity or over large surface area to become more violent than just rupturing any confinement. While burning rates are important, high-strain mechanical properties are nearly so, either by reducing existing porosity or generating additional surface area through fracture. The first example is deflagration-to-detonation transition (DDT) in porous beds. During the early stages, weak compressive waves ahead of the convective ignition front will reduce porosity, thereby restricting the spread of combustion and the pressure buildup. If, however, pressure increases faster than can be relieved by loss of confinement, coalescing compressive waves can initiate reaction at hot spots from rapid pore collapse. This compressive reaction can drive a shockwave that transits to detonation, the most violent reaction in any scenario. It has been shown that reaction violence is reduced in DDT experiments if the binder is softened, either by raising the initial temperature or adding a solvent. An example of the role of mechanical properties in enhancing reaction violence through fracturing occurs when cavities in projectile fills collapse during acceleration in the gun barrel, which is referred to as setback. Explosives with soft rubber binders will deform and undergo mild reaction from shear heating within the explosive and adiabatic compression of any gas in the cavity. Stiff explosives are similarly ignited, but also fracture and generate additional surface area for a violent event. The last example to be considered is slow cook-off, where thermal damage can increase burning rate as well as provide porosity to enhance the pressure buildup. As reaction spreads from the zone of thermal run-away, an explosive binder that resists breakup will limit the violence.

11:00AM V6.00002 ABSTRACT WITHDRAWN

11:15AM V6.00003 Thermal properties of a UK PBX and binder system. STEWART PALMER, DAVID WILLIAMSON, WILLIAM PROUD, University of Cambridge — The thermal conductivity, diffusivity and heat capacity of a UK PBX and binder system have been measured over a temperature range of ambient to approximately 120 °C. Independent measurements of any two of the above, and knowledge of the density, allows the third to be calculated. Comparisons between the directly measured and calculated values give an indication of the reliability of such data. Thermal conductivity measurements were made using the Lee’s disc method, thermal diffusivity via Ångström’s method and heat capacity via Differential Scanning Calorimetry (DSC). Such data are required for the development and validation of PBX thermal models. This paper outlines the current state of research and details the important observations to date.

11:30AM V6.00004 Critical Temperature Formula for a Body of Arbitrary Size and Shape. LARRY HILL, Los Alamos National Laboratory — The Frank-Kamenetskii thermal explosion model provides a framework for calculating the critical temperature for an energetic material body of any size and shape. The calculation involves finding a dimensionless shape parameter, which, except for the case of an infinite cylinder, must be determined numerically. This exercise is easy enough for simple symmetric geometries such as the infinite slab, infinite cylinder, and sphere, and these results are well known. But for arbitrary bodies the manipulations are cumbersome, to the extent that they are almost never undertaken in practice. It is therefore desirable to deduce a formula that can, to a good approximation, predict the critical temperature of an arbitrary body without the necessity of a heat transfer calculation. Over the past ~60 years, several attempts to find a universal formula have been made—none of which have been completely successful. It is not too difficult to develop a methodology that can reproduce the shape factor of the three canonical objects—infinite slab, infinite cylinder, and sphere. The challenge is to develop a methodology, which, while reproducing the three canonical objects, can also correctly distinguish the shape factors of, say, the sphere, cube, and a unity aspect ratio cylinder. I will present a method that can do so.

11:45AM V6.00005 Burn Propagation in a PBX 9501 Thermal Explosion. BRYAN HENSON, LAURA SMILOWITZ, JERRY ROMERO, Chemistry Division, LANL, BLAINE ASAY, MARY SANDSTROM, DE Division, LANL, PRAD COLLABORATION — We have measured burn velocities in a series of radially heated PBX 9501 thermal explosion experiments. Burn fronts have been imaged in these experiments using proton radiography. The velocities observed imply a convective burn front moving at approximately 200m/s. A compendium of burn velocities verses pressure show two distinct burn mechanisms: convection and conduction. The 200m/s velocity places the PBX 9501 radial thermal explosion experiment in the convective regime with an implied pressure on the order of 1 Gpa. The density evolution observed shows that HE continues to be consumed behind the convective front. The HE consumption follows the approximate radial symmetry of the heating profile. A hypothesis for the material consumption is made based on the implied pressures and material state. Implications for incorporating PBX 9501 thermal ignition and burn into larger scale models are discussed.
Non-random Crack Opening in Partially-Confined, Thermally-Damaged PBX 9501 and Observations on its Effects on Combustion, GARY PARKER, BLAINE ASAY, PETER DICKSON, PHILIP RAE, AXINTE IONITA, Los Alamos National Laboratory — During thermal insult to PBX 9501, damage in the form of cracking has been shown to modify the combustion mode and violence after ignition, since flames can intrude at lower pressures through cracks than the more tortuous matrix porosity. However, for fluid transport processes, including volumetric combustion and gas permeation, to occur the porosity must be open and accessible to the surfaces of the charge. Because many charges are encased (confined), there are mechanical limitations on the extent to which thermally-induced cracks can open, therefore diminishing their effect on transport to some concomitant extent. In this work, we present evidence for how strong radial confinement can result in aligned crack opening, despite the existence of plentiful randomly-oriented, though apparently closed, cracks. We damage cylinders in tight-fitting glass or metal sleeves open on both ends and observe the occurrence of preferential crack-opening normal to the cylindrical axis. This geometry and confinement is common in experimental arrangements such as strand burners and DDT tubes. Further, we observe, with high speed photography, how this non-random crack opening affects combustion and propose a mechanism, garnered from linear elastic finite element modeling, for why it occurs.