8:00AM A25.00001 Instability of planar detonation front in energetic materials MIKALAI BUDZEVICH, VASILY ZHAKHOVSKY, AARON LANDERVILLE, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — Detonation wave propagation in solid energetic materials (EMs), as described by the standard AB model, was studied using a novel moving window molecular dynamics (MW-MD) technique. Parameters of the AB model were modified to investigate the mechanisms of detonation propagation in EMs as a function of the activation barrier for the chemical reaction AB+B -> A+BB + + 3 eV. For barriers below 0.2 eV, the detonation front structure remained planar regardless of the cross-section of the sample. For higher activation barriers, the one-dimensional planar detonation evolves into a cellular detonation upon increase of one of the transverse dimensions of the sample. The cellular detonation transfers into a stable three-dimensional two-shock-like detonation upon simultaneous increase of both transverse dimensions of the sample. These various instabilities of the planar detonation front in solid EMs observed in our MW-MD simulations mirror the major regimes of gas-phase detonation, thus confirming the universal nature of detonation phenomena.

Monday, February 27, 2012 8:00AM - 11:00AM
Session A25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Energetic Materials 257A

8:12AM A25.00002 Shock-induced chemical reactions in organic materials and explosives DANA DATTELBAUM, STEPHEN SHEFFIELD, SHAWN MCGRANE, PETER GOODWIN, Los Alamos National Laboratory, SHOCK AND DETONATION PHYSICS TEAM — Interrogating chemical reactions behind a shock front is immensely difficult and, as a result, the details of shock-induced chemistry remain poorly understood. Previous research has shown that dimerizations, polymerizations, ring-opening and decomposition reactions can occur under shock compression, depending on molecular structure. Questions regarding the thresholds for incipient reaction, the nature of first and subsequent reaction steps, and the influence of shock input conditions on reaction kinetics remain to be answered. Here, we have applied in-situ electromagnetic gauging at multiple Lagrangian positions to elucidate the evolution of multiple-wave structures associated with shock-induced reactions of several simple functional groups: carbon-carbon double (C=C) and triple bonds, and nitriles. The relative order of group reactivity under single shock conditions for these simple molecules is discussed. From measurements of the reactive flow, we have obtained detailed information about the temporal evolution of the waves, and global kinetic rates associated with transformation(s) between partially- and fully-reacted states. Near the reactive thresholds, evolution in particle velocities point to reaction timescales on the order of tens-to-hundreds of nanoseconds. We further compare evidence of reaction from gas gun-driven experiments to recent results using laser-driven shocks. Spectroscopic details will be presented from both types of experiments.

8:24AM A25.00003 Molecular dissociation under extreme conditions IGOR SCHWEIGERT, US Naval Research Laboratory — Molecular dissociation under extreme temperatures and pressures is the first step towards thermal or shock initiated decomposition of energetic materials. Fast dissociation rates are challenging to measure, but amenable to first principles calculations. We combine transition-state theory with molecular dynamics simulations based on density-functional theory to predict the temperature-dependent dissociation rates in the gas and the condensed phase. Current applications focus on gas-, solution-, and liquid-phase thermal dissociation of nitramines. These studies will be discussed in the context of developing mesoscale models of initiation of energetic materials.

8:36AM A25.00004 Thermodynamic Properties of energetic materials from density functional theory with van der Waals corrections AARON LANDERVILLE, University of South Florida, MICHAEL CONROY, Naval Research Laboratory, MIKALAI BUDZEVICH, YOU LIN, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — The calculation of thermodynamic properties for energetic materials from first-principles offers the promise to provide key parameters for mesoscopic and continuum-level simulations of explosives performance for a wide range of pressures and temperatures. While density functional theory with empirical van der Waals corrections, together with corrections for temperature and zero-point effects, can give excellent agreement between calculated and experimentally determined equations of state, quantities such as heat capacities and coefficients of thermal expansion suffer from inaccuracies in the lower frequencies of the calculated vibration spectrum. Additional approaches are discussed to account for the lowest intermolecular modes to increase the accuracy in prediction of thermal properties.

8:48AM A25.00005 Relating polymorphism and decomposition of RDX under static and dynamic compression ZBIGNIEW DREGER, YOGENDRA GUPTA, Institute for Shock Physics, Washington State University — Knowledge of the reactive behavior of energetic crystals at static high pressures and high temperatures (HP-HT) is an important step toward understanding the shock wave initiation of these crystals. Vibrational spectroscopy in a diamond anvil cell was used to examine the behavior of RDX crystals at the pressures and temperatures relevant to shock wave initiation. Phase boundaries between three RDX polymorphs (α, γ, and ε) were determined up to 12 GPa and 600 K. Decomposition kinetics for the γ- and ε-phases were examined at various pressures and temperatures, and were found to have positive volumes of activation. CO₂, N₂O and H₂O were identified as the main decomposition species. Static HP-HT results were used to identify and understand the following processes in shocked RDX: α --> γ phase transition, identification of the crystal phase at decomposition, and the role of pressure and temperature in accelerating the RDX decomposition under shock compression. This work demonstrated that static HP-HT results provide an important complementary route to elucidate the physical and chemical processes in shocked RDX crystals.

9:00AM A25.00006 Atomic Simulations of Orientation and Shock Velocity Dependences on Pentanitrotetrazolium Tetranitrate Detonation Tzu-Ray Shian, Aidan T. Thompson, Ryan Wixon, Ann Mattsson, Sandia National Laboratories, Albuquerque, NM 87185, SANDIA TEAM — Predicting the behavior of energetic materials requires a detailed description of how chemical reaction, energy and pressure fronts propagate during initial stages of detonation. In this talk, classical molecular dynamics (MD) simulations are used to examine orientation and shock velocity dependences in single crystal pentanitrotetrazolium tetranitrate (PETN). This work utilizes an empirical, variable charge reactive force field (ReaxFF) that is implemented in the LAMMPS package with a time-averaged bond-order method for on-the-fly chemical species identification. The accuracy of ReaxFF is validated by comparisons of activation barriers for dissociation of a single PETN molecule along various dissociation channels with higher-fidelity, but more expensive density functional theory (DFT) calculations. The response of single-crystal PETN to shock compression is simulated using the multi-scale shock technique (MSST) along the insensitive (100) directions, as well as the sensitive (001) and (110) directions, at steady shock velocities ranging from 6-10 km/s. Hugoniot curves, particle velocities of shocked molecules, and evolution of reaction products with time from MD simulations with ReaxFF will be discussed and compared to that from DFT calculations.

This work is supported by DOE/NNSA and ONR/MURI.
9:12AM A25.00007 Atomic-Scale Theoretical Studies of Energy Transfer, Inelastic Deformation, and Void Collapse in Molecular Crystals and Polymers, THOMAS D. SEWELL, Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211 — Recent atomic-scale theoretical studies of shock waves in polyatomic molecular crystals and polymers will be presented, with an emphasis on the results and interpretation of molecular dynamics simulations for pentaerythritol tetranitrate (PETN), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), nitromethane, and poly(butadiene) (PBD). The effects of structural and mechanical anisotropy on the material response are of particular interest. Among the topics to be discussed are orientation dependent energy transfer pathways and inelastic deformation mechanisms subsequent to shock wave passage in initially defect-free nitromethane and PETN crystals, shock-induced collapse of variously shaped voids in crystalline RDX, and details of shock wave propagation and energy localization in bulk PBD and at the PBD/RDX interface.

9:48AM A25.00008 Explosive initiation of pentaerythritol tetranitrate (PETN) by laser irradiation, ROMAN TSYSHKEVSKYI, ONISE SHARIA, MAIJA KUKLJA, Materials Science and Engineering Department, University of Maryland, College Park, MD — Understanding of explosive decomposition of energetic materials triggered by laser irradiation is of great importance for design of new economical formulations with high performance and tunable sensitivity. Earlier, laser irradiation was only considered as a source of heat. Nowadays, it is realized that optical excitation may set off initiation of rapid chemical reactions and govern further decomposition in energetic materials. However, mechanisms of this phenomenon are yet to be established. We present quantum-chemical calculations of the electronic structure of molecular and crystalline PETN to explore the effect of common impurities on its optical properties. We found that charged or excited PETN molecules exhibit significantly different electronic, optical, and chemical behavior. For example, new decomposition pathways that were not available in the ground state become favorable in the charged state of PETN.

10:00AM A25.00009 Condensation of carbon during high explosive detonation, LAURENCE FRIED, SORIN BASTEA, RAUL GARZA, Lawrence Livermore National Lab — The formation of nano-carbon clusters is believed to be responsible for the non-ideal detonation behavior of carbon-rich explosives, such as triamino-trinitrobenzene (TATB). We have developed a new model of carbon formation during detonation. The model is based on the assumption that carbon cluster growth has features of both activated Arrhenius kinetics and diffusion controlled kinetics. In our model the variation of temperature, density, and viscosity throughout the high explosive reaction zone and expansion is calculated using a thermochemical model linked to a hydrodynamic code. We compare our model to new experimental results on the size scaling of detonations in TATB-based explosives.

10:12AM A25.00010 Surface-induced effect on sensitivity of beta and delta HMX crystals, ONISE SHARIA, MAIJA KUKLJA, Department of Materials Science and Engineering, University of Maryland, College Park — It is accepted that sensitivity of energetic materials depends on many factors, including presence of defects, surfaces, interfaces, or voids. However, details of atomistic mechanisms that govern sensitivity to initiation of detonation and correlations between structure, morphology, and degradation of chemical bonds are far from being understood. In this talk, we present quantum chemical calculations combined with transition state theory to analyze chemical decomposition reactions in beta and delta HMX crystals. We calculate the activation barriers and reaction rates in the ideal crystals and materials containing internal surfaces, vacancies, and voids. We show that N-NO\textsubscript{2} homolysis is the most favorable decomposition reaction in all cases. We discuss whether a large space available in the vicinity of voids facilitates the N-NO\textsubscript{2} break in comparisons to an ideal crystal, and if this effect is enhanced in the delta phase in comparison to beta phase. The conclusions and revealed trends are presented in the context of experimental data.

10:24AM A25.00011 ABSTRACT WITHDRAWN —

10:36AM A25.00012 1,1-Diamino-2,2-Dinitroethylene Under High-Pressure-High-Temperature\textsuperscript{1}, MATTHEW BISHOP, University of Alabama at Birmingham, NENAD VELISAVLJEVIC, Los Alamos National Laboratory, ZHENXIAN LIU, Carnegie Institution of Washington, MATRIN GALLEY, University of Nevada Las Vegas — 1,1-Diamino-2,2-dinitroethylene (FOX-7) is an insensitive high explosive (IHE) which shows promise for use in low vulnerability ammunitions. With performance comparable to RDX and HMX, there is a growing interest in understanding the behavior under detonation conditions. Through the use of diamond anvil cell (DAC) technology and electrical resistive heating, the vibrational behavior of FOX-7, in both the mid and far-IR, were recorded at multiple isotherms under elevated pressure-temperature (PT). Energy-dispersive x-ray diffraction (XRD) was also employed along with a multi-anvil press for further investigating pressure-temperature phase space. Future planned experiments will focus on using high-resolution angular-dispersive XRD and neutron diffraction techniques to resolve high pressure-temperature structural information and obtain P-V-T data. The experiments on FOX-7 have revealed previously uninvestigated knowledge on the elevated-PT decomposition and phase boundaries allowing for a more developed basis for the behavior of FOX-7 under detonation conditions.

\textsuperscript{1}Los Alamos National Laboratory (LANL) is operated by Los Alamos National Security (LANS), LLC for the Dept. of Energy and National Nuclear Safety Admin. Support for this research was provide by DOE/NNSA Science Campaign 2 under the HE Science Program.

10:48AM A25.00013 Study on the deflagration-to-detonation transition course of porous energetic material, LAN WEI, PENGCHENG HAO, HEFEI DONG, XIAOMIAN HU, JIANSHI ZHU, Institute of Applied Physics and Computational Mathematics — The deflagration-to-detonation transition (DDT) course of energetic material with different porosity ratio was studied utilizing a one-dimensional two-phase flow code. The equations were numerically solved by space-time conservation element and solution element (CE/SE) method. The effects of structural and mechanical anisotropy on the material response are of particular interest. Among the topics to be discussed are orientation dependent energy transfer pathways and inelastic deformation mechanisms subsequent to shock wave passage in initially defect-free nitromethane and PETN crystals, shock-induced collapse of variously shaped voids in crystalline RDX, and details of shock wave propagation and energy localization in bulk PBD and at the PBD/RDX interface.


NIR GOLDMAN, Lawrence Livermore National Laboratory — We report here on density functional tight binding (DFTB) simulations of covalently bonded materials over a pressure range of 10 – 2,000 GPa and a temperature range of 300 – 30,000 K using both standard and new interaction potentials we have created for these conditions. Density Functional Theory (DFT) has been shown to accurately reproduce the high pressure-temperature chemistry, phase boundaries, and EOS of many materials. DFT-MD simulations, though, scale poorly with computational effort and thus are generally limited to nanometer system sizes and picosecond time-scales. In contrast, chemical kinetic effects and phase changes can span up to nanosecond timescales and significantly longer length scales. The DFTB method holds promise as a high throughput simulation capability by providing orders of magnitude increase in computational efficiency while retaining most of the accuracy of Kohn-Sham DFT. We show that DFTB interaction potentials can be created by (a) fitting the DFTB repulsive energy to measured and computed compression data, and (b) using an extended basis set that includes d-orbital interactions, as needed. Our new potential for carbon yields accurate material properties for diamond, graphite, the BCB phase, and simple cubic carbon, as well as for the shock Hugoniot of diamond compressed up to the conducting liquid. We also discuss simulations of the long-time scale reactivity of H2O2 under detonation conditions, and shock compression of astrophysical ice mixtures and the subsequent synthesis of prebiotic materials. Our results provide a straightforward method by which DFTB can be made to provide equations of state and long-time scale chemical kinetic data at a similar accuracy to standard quantum codes. Our approach could be extended to any number of materials related to geology and planetary science, including silicon, SiO2, and hydrocarbon systems.

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Research funded by DTRA Grant No. HDTRA1-10-1-0038.

11:51AM B25.00002 Pressure-induced Polymerization in Substituted Acetylenes

RAJA CHELLAPPA, DANA DATTELBBAUM, STEPHEN SHEFFIELD, Los Alamos National Laboratory — A fundamental understanding of shock-induced chemical reactions in organics is still lacking and there are limited studies devoted to determining reaction mechanisms, evolution of bonding, and effect of functional group substitutions. The fast timescale of reactions occurring during shock compression create significant experimental challenges (diagnostics) to fully quantify the mechanisms involved. Static compression provides a complementary route to investigate the equilibrium phase space and metastable intermediates during high pressure chemistry, although at a much slower timescale. In this study, we present our results from our ongoing high pressure in situ synchrotron x-ray diffraction and vibrational spectroscopy experiments on substituted acetylenes: tert-butyl acetylene [TBA: (CH3)3-C≡CH] and ethynyl trimethylsilane [ETMS: (CH3)3-SC≡CH]. We observed the onset pressure of chemical reactions (at room temperature) in these compounds is significantly higher in static compression (TBA: 11 GPa and ETMS: 26 GPa) when compared to shock input pressures (TBA: 6.1 GPa and ETMS: 6.6 GPa). The products were polymeric in nature, recovered to ambient conditions with little degradation and fully characterized using spectroscopy, calorimetry, and other techniques to identify reaction mechanisms.

12:03PM B25.00003 Non-equilibrium Molecular Dynamics Studies of Interfacial Chemistry in Shocked Ni/Al Nanolaminates

JASON QUENNEVILLE, Spectral Sciences, Inc., NARESH THADHANI, Georgia Institute of Technology — The response of Ni/Al composite materials to shock loading has been studied using non-equilibrium molecular dynamics and an EAM force field. The simulation cells consist of layered Ni and Al laminates with at least 3 million particles in a 1:1 mole ratio. The main thrust of our research is to gain a better understanding of the chemistry that occurs at the Ni/Al interface when the real material is shocked. Initial geometries were chosen so as to identify the factors important to reaction in the complex macro-scale material. Specifically, we vary the orientation of the interface with respect to the shock wave and the geometry of the interface (i.e., deviation from planarity) to study how mixing and reactivity of Ni and Al are affected. Our results show a clear dependence of pressure and temperature on interface orientation, in agreement with continuum-scale simulations.

12:15PM B25.00004 Nearly Equivalency of Inter and Intramolecular Hydrogen Bonding Under High-Pressure

M. RIAD MANAA, LAURENCE FRIED, Lawrence Livermore National Laboratory — Triamino-trinitro-benzene (TATB, C6H6N6O6) exhibits unusually strong intramolecular hydrogen bonding as evidenced by the high rotational energy barrier of the nitro and amino groups. In the condensed phase, the competing intermolecular hydrogen bonding is pronounced at high pressure in its graphitic-like crystal structure. We report density functional theoretical calculations of the equation of state of TATB under hydrostatic compression of up to 250 GPa. Our results show our results show increasing bond equivalency between the intramolecular and intermolecular hydrogen bonds of the amino and nitro groups in the region 30<P<70 GPa, beyond which the difference between the two bond distances remains meaningful. This is manifested by a rapid decrease of the intermolecular NO–HN– NO–HN– bond distance along the b lattice direction from 2.6 Å at the zero pressure equilibrium geometry to 1.72 Å at 67 GPa, and by a decrease of the intramolecular NO–HN– bond from 1.65 Å to 1.57 Å for the same pressure region. It is expected that vibrational motions involving the NO–HN modes are sensitive to the nearly equivalent hydrogen bonding, as recent spectroscopic IR analysis of the NH2 stretches revealed.

12:27PM B25.00005 Modeling of electron-ion coupling in shocked materials

EVAN REED, Stanford University — This work describes and implements a quasi-statistical approach to electron-ion coupling in shocked matter. By combining this approach with the multi-scale shock technique (MSST) and a tight-binding model, the magnitude and role of electronic excitations in shocked energetic materials are studied theoretically using quantum molecular dynamics simulations. Focusing on the detonating primary explosive HN3 (hydrazoic acid), this work finds that the material transiently exhibits a high level of electronic excitation characterized by carrier densities in excess of 10^18 cm^-3, or one electronic excitation for every 8 molecules. Electronic excitations enhance the kinetics of chemical decomposition by about 30%. The electronic heat capacity has a minor impact on the temperatures exhibited, on the order of 100 K.

12:39PM B25.00006 Quantum-based Molecular Dynamics Simulations of Shock-induced Reactions with Time-resolved Raman Spectra

MARC CANKWELL, EDWARD SANVILLE, JOSHUA COE, ANDERS NIKLASSON, Los Alamos National Laboratory — Shock-induced reactions in liquid hydrocarbons have been studied using quantum-based, self-consistent tight-binding (SC-TB) molecular dynamics simulations with an accurate and transferable model for interatomic bonding. Our SC-TB code LATTE enables explicit simulations of shock compression using the universal liquid Hugoniot. Furthermore, the effects of adiabatic shock heating are captured precisely using Niklasson's energy conserving extended Lagrangian Born-Oppenheimer Molecular Dynamics formalism. We have been able to perform relatively large-scale SC-TB simulations by either taking advantage of the sparsity of the density matrix to achieve O(N) performance or by using graphics processing units to accelerate O(N^2) algorithms. We have developed the capability for the on-the-fly computation of Raman spectra from the Fourier transform of the polarizability autocorrelation function via the density matrix perturbation theory of Niklasson and Challacombe. These time-resolved Raman spectra enable us compare the results of our simulations with identical diagnostically collected experimentally. We will illustrate these capabilities with a series of simulations of shock-induced reaction paths in a number of simple molecules.
12:51PM B25.00007 Molecular Simulation of Shock Hugoniot for Polymers, T. SIRK, T. CHANTAWANSRI, E. BYRD, B. RICE, J. ANDZELM, Army Research Laboratory — The behavior of polymers under extreme conditions (high pressure and temperature) is of interest for a variety of applications, such as polymer-bonded explosives, coatings, adhesives, and light-weight armor. Material properties and response at extreme conditions can be determined through shock experiments, which are often difficult to measure experimentally because of difficulties in traversing a large range of pressures (up to hundreds of gigapascals) and temperatures (thousands of kelvin) with available instrumentation. In addition, interesting behavior, such as observed behind a shock front, occurs at extremely short time- and length-scales (nanoscale), which poses problems in characterizing the material using current experimental capabilities. To further understand shocked systems, simulation methods such as molecular dynamics (MD) and quantum mechanics (QM) can be used to provide insight into atomic-level phenomena. Using classical MD and QM, we have calculated the principle shock Hugoniot curves for four polymers: poly(methyl methacrylate), poly(ethylene), poly(styrene), and hydroxyl-terminated poly(butadiene). In the MD calculations, we considered both a non-reactive (i.e. PCFF) and reactive (i.e. ReaxFF) forcefield, respectively, where calculations were performed in LAMMPS. The QM calculations were performed with density functional theory (DFT) using dispersion corrections as implemented in CP2K. We have applied both atom centered pseudopotentials (DCA-p) and Grimme van der Waals corrections in our study. Overall, results obtained by QM show much better agreement with available experimental data for the range of up to 20 GPa than classical force fields. At pressures where reactions can occur the short simulation time available in MD modeling prevents us from fully exploring possible reaction pathways.

1:03PM B25.00008 Amorphous Polymeric Nitrogen from Dynamic Shock Simulation¹, TODD BEAUDET, WILLIAM MATTSON, BETSY RICE, U.S. Army Research Laboratory — In recent years there has been significant interest in polymeric phases of nitrogen at low pressure for potential application as an energetic material. This interest was bolstered by experimental evidence of metastable amorphous polymeric nitrogen at low pressure.² While considerable theoretical work has been done on many crystal phases of nitrogen, simulating amorphous polymeric nitrogen has been more challenging. Starting from first principles dynamic shock simulation of cubic-gauche nitrogen,³ we demonstrate a form of polymeric nitrogen at low pressure that may be directly related to amorphous polymeric nitrogen.

¹This research was supported in part by an appointment to the U.S. Army Research Laboratory Postdoctoral Fellowship Program administered by the Oak Ridge Associated Universities through a contract with the U.S. Army Research Laboratory.

1:15PM B25.00009 ABSTRACT WITHDRAWN —

1:27PM B25.00010 Ethane and Xenon mixing: density functional theory (DFT) simulations and experiments on Sandia’s Z machine, RUDOLPH MAGYAR, SETH ROOT, THOMAS MATTSSON, KYLE COCHRANE, Sandia National Laboratories — The combination of ethane and xenon is one of the simplest binary mixtures in which bond breaking is expected to play a role under shock conditions. At cryogenic conditions, xenon is often understood to mix with alkanes such as Ethane as if it were also an alkane, but this model is expected to break down at higher temperatures and pressures. To investigate the breakdown, we have performed density functional theory (DFT) calculations on several xenon/ethane mixtures. Additionally, we have performed shock compression experiments on Xenon-Ethane using the Sandia Z – accelerator. The DFT and experimental results are compared to hydrodynamic simulations using different mixing models in the equation of state. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of the Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:39PM B25.00011 Dynamic Response of a Carbon Fiber – Epoxy Composite, SCOTT ALEXANDER³, WILLIAM REINHART, Sandia National Laboratories — The dynamic response of carbon fiber reinforced epoxy composite materials was investigated under planar impact loading. The samples were unidirectional (all carbon fibers oriented in a single direction) with fiber fill volumes from 62 to 68%. Gun driven planar impact tests with impact velocities of 0.1-2.0 km/s were conducted allowing samples to be compressed up to about 15 GPa. Velocity interferometry was used to measure particle velocities from which the compressed state of the samples was determined. Wave speeds for shocks traveling along the carbon fibers are significantly higher than for those traveling transverse to the fibers or through the bulk epoxy. As a result, the dynamic material response is dependent on the relative shock – fiber orientation. Shocks traveling along the fiber direction exhibit both elastic and plastic characteristics over the stress range tested. Shocks traveling transverse to the fibers show only a single wave response similar to but slightly stiffer than the bulk response of the epoxy. Results will be presented detailing these findings which provide a basis for modeling this class of directional composite materials.

¹Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
²This work was performed under the auspices of the US Dept. of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.
³Tomorr HAXHIMALI, ROBERT RUDD, Lawrence Livermore National Laboratory — We employ classical molecular dynamics (MD) to estimate species diffusivity and viscosity in binary Yukawa Mixtures. The Yukawa potential is used to describe the screened Coulomb interaction between the ions, providing the basis for models of dense static materials, inertial confined plasmas, and colloidal particles in electrolytes. We calculate transport coefficients in equilibrium simulations using the Green-Kubo relation over a range of thermodynamic conditions including the viscosity and the self-diffusivity for each component of the mixture. The inter-diffusivity (or mutual diffusivity) can then be related to the self-diffusivities by using a generalization of the Darken equation. We have also employed non-equilibrium MD to estimate inter-diffusivity during the broadening of the interface between two regions each with a high concentration of either species. The main motivation in this work is to build a model that describes the transport coefficients in binary Yukawa mixtures over a broad range of thermodynamic conditions.

1:51PM B25.00012 Calculation of Transport Coefficients in Binary Yukawa Mixtures¹, TOMORR HAXHIMALI, ROBERT RUDD, Lawrence Livermore National Laboratory — We employ classical molecular dynamics (MD) to estimate species diffusivity and viscosity in binary Yukawa Mixtures. The Yukawa potential is used to describe the screened Coulomb interaction between the ions, providing the basis for models of dense static materials, inertial confined plasmas, and colloidal particles in electrolytes. We calculate transport coefficients in equilibrium simulations using the Green-Kubo relation over a range of thermodynamic conditions including the viscosity and the self-diffusivity for each component of the mixture. The inter-diffusivity (or mutual diffusivity) can then be related to the self-diffusivities by using a generalization of the Darken equation. We have also employed non-equilibrium MD to estimate inter-diffusivity during the broadening of the interface between two regions each with a high concentration of either species. The main motivation in this work is to build a model that describes the transport coefficients in binary Yukawa mixtures over a broad range of thermodynamic conditions.

²This work was performed under the auspices of the US Dept. of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

2:03PM B25.00013 Fracture of Constructional Materials with the Covering at Shock-Wave Loadings, PAVEL RADCHENKO, Institute of Strength Physics and Materials Science SB RAS, Russia, ANDREY RADCHENKO, Tomsk State University of Architecture and Building, Russia — The behavior of constructional materials with a covering subjected to shock load is numerically modeled. The covering on a material is applied by the method of high velocity oxygen fuel. The materials created by a similar method, are widely applied in aerospace branch, both for creation of engines and for creation of details of cases. Possibility of application of multilayered coverings essentially expands the spectrum of researches for the analysis of separate layer influence on behavior of a design as a whole. Features of behavior of this sort of materials is an actual problem as well as construction of authentic models of behavior of materials with coverings as a whole. Influence of a material of a covering, quantity of layers and their geometrical parameters on fracture and shock-wave processes in a material is investigated. The range of velocities of interaction from 50 to 2000m/sec is considered. As projectiles steel cylinders and spheres were used.
Monday, February 27, 2012 2:30PM - 5:06PM –
Session D25 DCOMP GS4CM DMP: Focus Session: Matter at Extreme Conditions - New Experimental Capabilities 257A

2:30PM D25.00001 Ultrafast, high resolution, phase contrast imaging of shock response with synchrotron radiation: opportunities and challenges, S.N. LUO, B.J. JENSEN, D.E. HOOKS, K.J. RAMOS, J.D. YEAGER, K. KWIATKOWSKI, T. SHIMADA, D.A. FREDENBURG, Los Alamos National Lab, K. FEZZAA, Argonne National Lab — Designing materials that function at dynamic extremes and predicting dynamic materials response require experimental investigations of their time, rate and microstructure dependences. Key to such experiments are in situ, in-volume, temporally and spatially resolved measurements (e.g., x-ray imaging and diffraction). Here we report ultrafast (<100 ps), high resolution (~3 μm), dynamic phase contrast imaging (PCI) measurements during high strain-rate loading (100 ns scale). A gas gun was installed at 32ID beamline of the Advanced Photon Source for dynamic loading, and dynamic PCI measurements were performed with a single x-ray pulse on representative materials/processes, including cylinder impact and penetration, large-cell foam compaction, cerium jet formation and granular material compression. We present overall experimental scheme and opportunities for dynamic materials research as seen from the preliminary results, as well as challenges both for photon sources and detectors.

2:42PM D25.00002 Probing Matter at an Atomic Unit of Pressure using convergent compression, JAMES HAWRELIAK, DAMIAN SWIFT, JON EGGERT, DAVE BRAUN, LLNL, STEVE ROTHMAN, AWE, GILBERT COLLINS, LLNL — Geometric confinement significantly increases the shock pressure as a spherically-converging shock approaches the central focus. Inertial confinement fusion is one area where this technique enables the 100 MBar ablation pressure to multiply to the several-GBar pressure required for fusion. We are using x-ray radiography of a spherically convergent shock wave in a solid sphere to explore material equations of state at pressures which exceed the atomic unit of pressure (Eh/a0 = 300 MBar); the energy density of a hydrogen atom. Measuring materials properties above this pressure will breach yet another significant barrier in our quest to understand extreme states, and will open a completely new realm where the atomic nature of matter is very strongly perturbed. We will discuss initial experiments preformed on the Omega laser facility and plans for future experiments on the NIF.

3:06PM D25.00004 Deformation and material dynamics under ultrafast compression, MICHAEL ARMSTRONG, Lawrence Livermore National Laboratory — For decades, dynamic compression experiments have been used to determine the equation of state of materials, and examine material deformation at high strain rates. Within the last 15 years, ultrafast optical methods have been used to characterize deformation at strain rates in excess of 10^10/s. Recently such experiments have found broad consistency with empirical laws formulated at orders of magnitude lower strain rates, but have also discovered intriguing phenomena on short time scales, such as elastic stress orders of magnitude beyond the yield strength. These experiments explore the ultimate limits of material relaxation via deformation, and the results suggest exciting possibilities for practical and scientific application of ultrafast compression, including nonequilibrium material synthesis, determination of the equation of state with a small scale experiment, and the investigation of ultrahigh density with a table top laser. Here we will talk about our experiments on the ultrafast deformation of metals, including aluminum and iron, and the ultrafast compression of deuterium.

3:42PM D25.00005 High-resolution phase contrast imaging of jet formation in shocked cerium to examine material strength, BRIAN JENSEN, SHENG LUO, FRANK CHERNE, GUY DIMONTE, GUILLERMO TERRONES, DANIEL HOOKS, KYLE RAMOS, JOHN YEAGER, KRIS KWIATKOWSKI, TSUTOMU SHIMADA, Los Alamos National Laboratory, KAMEL FEZZAA, Advanced Photon Source — Heterogeneous processes involved in brittle failure necessitate in situ, spatially resolved observation. An impact capability has recently been developed within which synchrotron phase contrast imaging (PCI), at the 32-ID beamline of the Advanced Photon Source, can be used to resolve crack interfaces during dynamic deformation. The imaging is both fast and high-resolution as images with approximately 3 micrometer resolution are obtained from single x-ray pulses (<100 ps duration). Experiments have been performed to investigate questions regarding velocimetry interpretation, the effect of stress states, and whether cracking can occur under uniaxial compression. Uniaxial compression and tension in planar impact configurations and cylindrical impact penetration has been used to vary stress states and observe failure. PCI and velocimetry results from these experiments will be presented for a range of brittle materials spanning glasses and ceramics.

3:54PM D25.00006 High-resolution phase contrast imaging for simultaneous Measurements of Velocity and Density in Shock-Driven Instabilities, RICARDO MEJIA-ALVAREZ, SRIDHAR BALASUBRAMANIAN, GREG ORLICZ, KATHY PRESTIDGE, Los Alamos National Laboratory — The interaction between a shock wave and the interface between two fluids of different density might induce macroscopic mixing of the fluids. It is generally accepted that baroclinic vorticity, resulting from misalignments between the density gradient across the interface and the pressure gradient of the shock wave, impels this macroscopic mixing. So far, the Extreme Fluids Team at Los Alamos National Laboratory has conducted the only detailed studies of the structure of the developing instability. These studies encompass simultaneous measurements of velocity and density via combined Particle Image Velocimetry (PIV) and Planar Laser Induced Fluorescence (PLIF). Using this approach, the above mentioned Team has conducted extensive studies over a varicose curtain of heavy gas (SF6). Since a curtain implies two succeeding interfaces, a new Vertical Shock Tube (VST) was developed for simultaneous characterization of velocity and density fields of single-interface shock-driven flows. This talk is intended to present some of the results obtained for double-interface shock driven flows, as well as describing the characteristics, challenges, and range of possibilities of the laser diagnostics incorporated in the VST.
and rise times. From these data, we directly validate


4:18PM D25.00008 Progress towards Single Shot Spectroscopic Techniques for Time-Resolved Measurements in the Diamond Anvil Cell, DOUGLAS ALLEN DALTON, Geophysical Laboratory, Carnegie Institution of Washington, R. STEWART MCMILLIONS, M. F. MAHMOOD, Howard University and Geophysical Laboratory, ALEXANDER F. GONCHAROV, Geophysical Laboratory — We will discuss how we are bridging the gap between static diamond anvil cell and dynamic shock experiments using various spectroscopic techniques which utilize nonlinear optics. Using pulsed laser techniques, we can achieve extreme temperatures while probing optical and chemical changes on fast time scales. Recent developments incorporating broadband spectroscopy into the laser heated diamond anvil cell have indicated that probing phase transitions while measuring temperature is possible [1]. Various methods for incorporating nonlinear vibrational spectroscopy (such as CARS) into the diamond anvil cell will be discussed. The application of these optical diagnostics to pulsed laser heating and table-top shock experiments [2] will be presented.

1. R.S. McWilliams et al., in preparation.


4:30PM D25.00009 Phase diagram of shock and ramp-compressed tin, AMY LAZICKI, JONATHON EGGERT, RYAN RYGG, DAMIAN SWIFT, JAMES MCNANEY, GILBERT COLLINS, Lawrence Livermore National Laboratory — We will present powder x-ray diffraction results on laser-ramp-compressed solid tin up to 600 GPa, and discuss new methods for detecting the melting transition. Tin has a complex phase diagram with multiple observed and predicted high pressure phases and a moderate melting temperature, making it an ideal subject for a fundamental study of material properties using new techniques. Ramp compression in the solid allows access to extremely dense condensed phases and in the liquid the possibility for dynamically freezing molten tin. With newly developed x-ray diffraction methods we examine crystal structure, strength and texture in the dynamically compressed phases, and explore the possibility of a new method for mapping out melting curves.

4:42PM D25.00010 Ultrafast Shock Interrogation of Hydrogen Peroxide/Water Mixtures: Thermochemical Predictions of Shock Condition Chemistry1, JOSEPH ZAUG, MICHAEL ARMSTRONG, SORIN BASTEA, JEFFREY CARTER, I.-F. WILLIAM KUO, JONATHAN CROWHURST, CHRISTIAN GRANT, Lawrence Livermore National Laboratory, X-CHEM TEAM — Hydrogen peroxide is a powerful oxidizer and its concentrated aqueous solutions exhibit very high reactivity, even sustaining detonation under strong enough confinement. Due to its simple composition and basic expected decomposition kinetics hydrogen peroxide is very suitable for studying the interplay of high pressures, temperatures and reactivity and their effect on the equation of state, particularly at the boundary between detonating and non-detonating behavior. To this end we performed speed of sound and picosecond time resolved shock measurements on solutions of hydrogen peroxide of concentrations from 30 to 90 percent, and analyzed the results in terms of common assumptions of chemical equilibrium in reactive fluid mixtures. Experimental shock states were achieved up to a maximum pressure of 20 GPa with corresponding shock velocities of 6-7 km/sec.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344. We acknowledge the LLNL Laboratory Directed Research and Development office for support.

4:54PM D25.00011 Simulation of Forward and Inverse X-ray Scattering From Shocked Materials, JOHN BARBER, QUINN MARKSTEINER, CRIS BARNES, Los Alamos National Laboratory — The next generation of high-intensity, coherent light sources should generate sufficient brilliance to perform in-situ coherent x-ray diffraction imaging (CXDI) of shocked materials. In this work, we present beginning-to-end simulations of this process. This includes the calculation of the partially-coherent intensity profiles of self-amplified stimulated emission (SASE) x-ray free electron lasers (XFELs), as well as the use of simulated, shocked molecular-dynamics-based samples to predict the evolution of the resulting diffraction patterns. In addition, we will explore the corresponding inverse problem by performing iterative phase retrieval to generate reconstructed images of the simulated sample. The development of these methods in the context of materials under extreme conditions should provide crucial insights into the design and capabilities of shocked in-situ imaging experiments.

Tuesday, February 28, 2012 8:00AM - 11:00AM –
Session H25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Shock Compression of Metals 257A

8:00AM H25.00001 Invariance of the Dissipative Action at Ultrahigh Strain Rates above the Strong Shock Threshold1, JONATHAN CROWHURST, MICHAEL ARMSTRONG, KIMBERLY KNIGHT, JOSEPH ZAUG, ELAINE BEHYMER, Lawrence Livermore National Laboratory — We have directly resolved shock structures in pure aluminum in the first few hundred picoseconds subsequent to a dynamic load, at peak stresses up to 43 GPa and strain rates of in excess of 1014 s−1. For strong shocks we obtain peak stresses, strain rates, and rise times. From these data, we directly validate1 the invariance2 of the dissipative action in the strong shock regime, and by comparing with data obtained at much lower strain rates show that this invariance is observed over at least 5 orders of magnitude in the strain rate. Over the same range, we similarly validate the fourth-power scaling of strain rate with peak stress (the Swegle-Grady relation). 1. J. C. Crowhurst, M. R. Armstrong, K. B. Knight, J. M. Zaug, E. M. Behymer, Phys. Rev. Lett, 107, 144302 (2011). 2. D. E. Grady, J. Appl. Phys. 107, 013506 (2010). This work was also supported by the EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Grant No. DESC0001057.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 with Laboratory directed Research and Development funding (11ERD039)
metals will be presented employing semi-empirical potentials of the embedded atom method (EAM) type as well as results from density functional theory. The directional-dependence of the yield strength in single crystals is shown to be due to the onset of instabilities in elastic-wave propagation velocities. The generic characteristics: high elastic limits, large directional anisotropies in the yield stress and pre-melting much below the equilibrium melt temperature for shock unavailability or hard to measure experimentally. Computational studies of shock-induced plasticity and melting in fcc and bcc single, mono-crystal metals, exhibit high strain rates ($10^{9}$ s$^{-1}$).

University of Texas-El Paso — Large-scale non-equilibrium molecular dynamics (MD) simulations are now commonly used to study material deformation at compression at a wide range of strain rates ($10^{8}$ s$^{-1}$). They can provide detailed information—such as defect morphology, dislocation densities, and temperature and stress profiles, unavailable or hard to measure experimentally. Computational studies of shock-induced plasticity and melting in fcc and bcc single, mono-crystal metals, exhibit generic characteristics: high elastic limits, large directional anisotropies in the yield stress and pre-melting much below the equilibrium melt temperature for shock wave propagation along specific crystallographic directions. These generic features in the response of single crystals subjected to high strain rates of deformation can be explained from the changes in the energy landscape of the uniaxially compressed crystal lattice. For time scales relevant to dynamic shock loading, the directional-dependence of the yield strength in single crystals is shown to be due to the onset of instabilities in elastic-wave propagation velocities. The elastic-plastic transition threshold can accurately be predicted by a wave-propagation stability analysis. These strain-induced instabilities create incipient defect structures, which can be quite different from the ones, which characterize the long-time, asymptotic state of the compressed solid. With increase compression and strain rate, plastic deformation via extended defects gives way to amorphization associated with the loss in shear rigidity along specific deformation paths. The hot amorphous or (super-cooled liquid) metal re-crystallizes at rates, which depend on the temperature difference between the amorphous solid and the equilibrium melt line. This plastic-amorphous transition threshold can be computed from shear-waves stability analyses. Examples from selected fcc and bcc metals will be presented employing semi-empirical potentials of the embedded atom method (EAM) type as well as results from density functional theory calculations.

1 Part of this work was supported by the U.S. Department of Energy under contract DE-AC52-06NA25396.

2 Computational Physics Division, Los Alamos National Laboratory.
9:48AM H25.00008 Metallurgical Effects Upon the Shock Response of Tantalum: Cold Work and Dilute Alloying. JEREMY MILLET, AWE — The response of the body centred cubic metal tantalum to shock loading has been studied for several decades, due to its use by the military in explosively formed projectiles. It can also be considered as an ideal body centred cubic metal, thus rendering it ideal for studies of fundamental mechanical and microstructural behaviour. Previous studies on well controlled, annealed specimens has shown that deformation is controlled by the motion of rather than the generation of a/2{111}{100} screw dislocations in straight segments, which result in little if any post shock hardening. In situ-shape strength measurements have also shown a significant strength reduction behind the shock front, suggesting that the motion of these dislocations acts as a stress relief mechanism. Similar effects have also been noted in tungsten and its alloys, but very recently, measurements in niobium and molybdenum show shear strength to be near constant behind the shock front. Other factors, such as variation of Peierls stress effecting ease of dislocation generation and the propensity to twin also have a strong effect upon the shock response. In this presentation, we return to tantalum, investigating the differences in shock response between a low dislocation density (annealed) and high dislocation density (cold rolled) material. We also examine the effects of dilute alloying through the addition of 2.5 wt% tungsten to tantalum. Results are discussed in terms of the shear strength and its variation with time behind the shock front.

10:00AM H25.00009 High Strain Rate Behavior of Nanoporous Tantalum1. CARLOS J. RUESTES, Instituto de Ciencias Basicas, Univ. Nac. Cuyo, EDUARDO M. BRINGA, CONICET - Instituto de Ciencias Basicas, Univ. Nac. Cuyo, ALEXANDER STUKOWSKI, Lawrence Livermore National Laboratory, JOAQUIN F. RODRIGUEZ NIEVA, Massachusetts Institute of Technology, GRACIELA BERTOLINO, CONICET - Centro Atomico Bariloche, MARC A. MEYERS, University of California, San Diego — Nano-scale failure under extreme conditions is not well understood. In addition to porosity arising from mechanical failure at high strain rates, porous structures also develop due to radiation damage. Therefore, understanding the role of porosity on mechanical behaviour is important for the assessment and development of materials like metallic foams, and materials for new fission and fusion reactors, with improved mechanical properties. We carry out molecular dynamics (MD) simulations of a Tantalum (a model body-centered cubic metal) crystal with a collection of nanovoids under compression. The effects of high strain rate, ranging from 10^7 s^-1 to 10^9 s^-1, on the stress strain curve and on dislocation activity are examined. We find massive total dislocation densities, and estimate a much lower density of mobile dislocations, due to the formation of junctions. Despite the large stress and strain rate, we do not observe twin formation, since nanopores are effective dislocation production sources. A significant fraction of dislocations survive unloading, unlike what happens in fcc metals, and future experiments might be able to study similar recovered samples and find clues to their plastic behavior during loading.

1Research funded by PICT2008-1325, PICT2009-0092 and SeCyTY.

10:12AM H25.00010 High-Pressure Strength Determination via Quasi-Elastic Optimization Analysis. JUSTIN BROWN, TRACY VOGLER, JIM ASAY, Sandia National Laboratories — The analysis of unloading profiles from ramp wave experiments on Sandia’s Z machine for the purposes of extracting strength information can be greatly influenced by the presence of a window. An impedance mismatch between the sample and the window generates a reflected ramp wave which perturbs the incoming wave, particularly at later times when, during unloading, the material strength becomes evident. In an effort to analyze the waveforms for an accurate estimate of the strength, the experimental data is coupled with optimized numerical simulations. Simulations were performed with LASLO, a one-dimensional magneto-hydrodynamics code. The deviatoric response was calculated using a modified rate-independent Steinberg-Guinan model in which a quasi-elastic response was implemented during unloading by linearly varying the material strength becomes evident. In an effort to analyze the waveforms for an accurate estimate of the strength, the experimental data is coupled with optimized numerical simulations. Simulations were performed with LASLO, a one-dimensional magneto-hydrodynamics code. The deviatoric response was calculated using a modified rate-independent Steinberg-Guinan model in which a quasi-elastic response was implemented during unloading by linearly varying the shear modulus. A best fit of relevant parameters in this strength model along with the magnetic field at the drive surface were estimated over the course of thousands of simulations using the Dakota optimization package. These results may then be used to estimate the in situ wave profiles from which the strength can be extracted. Initial results will be presented for ramp wave compression of tantalum with a lithium fluoride window to peak stresses of ~120 GPa. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

10:24AM H25.00011 Calculation of diffusivity and viscosity of Al-Cu molten mixtures using molecular dynamics1. ROBERT RUDD, WILLIAM CABOT, KYLE CASPERSEN, JEFF GREENOUGH, TOMORR HAXHIMALI, PAUL MILLER, DAVID RICHARDS, FREDRIC STREITZ, Lawrence Livermore National Lab — We use equilibrium classical molecular dynamics and Green-Kubo techniques to calculate the diffusivity and viscosity of Al-Cu molten mixtures. We calculate both the self-diffusivities and the Maxwell-Stefan diffusivities, and evaluate the validity of the Green-Kubo relation for this system. We compare our results with those from experiments reported in the literature. We have constructed an analytic model that is fit to the MD results. This transport model has been implemented in a continuum hydrodynamics code. Both the continuum code and extremely large-scale molecular dynamics have been used to simulate the development of vortices due to the Kelvin-Helmholtz instability in a shear layer, and we discuss the results of that comparison.

1This work was performed under the auspices of the US Dept. of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

10:36AM H25.00012 Mechanical Behaviour of Light Metal Alloys at High Strain Rates. Computer Simulation on Mesoscale Levels. VLADIMIR SKRIPNYAK, EVGENIYA SKRIPNYAK, Tomsk State University, LOTHAR W. MEYER, NORMAN HERZIG, Nordmetall GmbH, NATALIYA SKRIPNYAK, Tomsk State University, TOMSK STATE UNIVERSITY TEAM, NORDMETALL GMBH TEAM — Researches of the last years have allowed to establish that the laws of deformation and fracture of bulk ultrafine-grained and coarse-grained materials are various both in static and in dynamic loading conditions. Development of adequate constitutive equations for the description of mechanical behavior of bulk ultrafine-grained materials at intensive dynamic influences is complicated in consequence of insufficient knowledge about general rules of inelastic deformation and nucleation and growth of cracks. Multi-scale computational model was used for the investigation of deformation and fracture of bulk structured aluminum and magnesium alloys under stress pulse loadings on mesoscale level. The increment of plastic deformation is defined by the sum of the increments caused by a nucleation and gliding of dislocations, the twinning, meso-blocks movement, and grain boundary sliding. The model takes into account the influence on mechanical properties of alloys an average grains size, grain sizes distribution of and concentration of precipitates. It was obtained the nucleation and gliding of dislocations caused the high attenuation rate of the elastic precursor of ultrafine-grained alloys than in coarse grained counterparts.

10:48AM H25.00013 Estimation of spectral characteristics of particles ejected from free surfaces of metals and liquids under shock wave effect. ALLA GEORGIEVSKAYA, VICTOR RAEVSKY, RFNC-VNIIEF — The authors present approximated relations for estimations of the basic characteristics of flow of particles ejected from free surface of substance after shock wave arrival (shock-wave ejecta). The problem is considered as a particular case of the Richtmyer-Meshkov instability. Periodic perturbations on free surface, which are sinusoidal and having triangular shape, are considered as the initial perturbations causing formation of jets and particles. The medium is assumed to be liquid with surface tension. The role of viscosity is estimated. In the work, the authors obtained equations for estimations of the following characteristics of the particle flow: - dependence of integral mass of ejected substance on time; - space-time distribution of density of ejected substance; - space-time distribution of velocity of ejected substance; - distribution of particles in sizes; - correlation of sizes and velocities of particles. Estimations are presented concerning influence of shear strength and plasticity on substance ejecta. Analytical relations are compared with results of numerical calculations and experiments.
11:15AM J25.00001 Single two-zone elastic-plastic shock waves in solids, VASILY ZHAKHOVSKY, MIKALAI BUDZEVICH, University of South Florida, NAIL INOGAMOV, Landau Institute for Theoretical Physics, Russian Academy of Sciences, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — A new regime of shock wave propagation in solids, corresponding to a single two-zone elastic-plastic shock wave, was discovered using a novel moving window molecular dynamics technique. Both leading low-pressure elastic and trailing high-pressure plastic fronts move with the same speed and have a fixed separation that can extend to several microns. The material in the elastic zone is in a metastable state, having a pressure that substantially exceeds the critical shock strength characteristic of the onset of the well-known split-elastic-plastic, two-wave regime. The single elastic-plastic shock wave is a quite general phenomenon observed in our simulations for a broad class of crystalline materials, including aluminum, nickel, diamond, and Lennard-Jones crystals. It is the existence of the two-zone, elastic-plastic regime that allows for a consistent explanation of the anomalously high elastic wave amplitudes observed in recent experiments.

11:27AM J25.00002 The Role of Shock Induced Defect Structure in Spall Failure, JUSTIN WILKERSON, K.T. RAMESH, The Johns Hopkins University — Spall failure is a complex multiscale, multirate process. On the macroscale the process involves a period of shock compression followed by dynamic tension set up by the stress wave interactions. During the shock compression, the material undergoes a myriad of shock stress magnitude and pulse duration dependent microscopic processes that may include dislocation multiplication, nucleation, trapping, pile-up, annihilation, recovery, cell evolution as well as vacancy generation and clustering. In addition to shock hardening the material, this new shock induced defect structure seeds the material with potential void nucleation sites that may be activated during the proceeding period of dynamic tensile loading. Upon nucleation, the voids undergo dynamic growth to coalescence, constrained by inertia and viscoplastic resistance to deformation. A multiscale predictive framework is developed to analyze the role of these time-dependent processes in the experimentally observed spall strength dependence on initial microstructure, preheated temperature, tensile loading rate, pulse duration, and shock stress magnitude.

11:39AM J25.00003 Physics of hyper-velocity impacts of micrometer and sub-micrometer sized particles, ANNA MOCKER, IRS, University of Stuttgart, Germany, KLAUS HORNUNG, Universitat der Bundeswehr Muenchen, Germany, ZOLTAN STERNOVSKY, KEITH DRAKE, SASCHA KEMPF, CCLLAS, University of Colorado at Boulder, EBERHARD GRUN, MPI-K, Heidelberg, Germany, FIEGE FIEGE, University of Heidelberg, Germany, Ralf SRAMA, IRS, University of Stuttgart, Germany — The phenomena occurring during hypervelocity microparticle impact are manyfold and the basis for the variety of applications. The processes of interest are particle fragmentation, impact ionization, impact flashes, and TOF mass spectrometry. To relate the parameters of individual particle impacts with the resulting measured values, a comprehensive program of impact experiments under well-known experimental conditions for a wide variety of impact parameters is needed. For this, dust particles are accelerated to hypervelocity speeds with an electrostatic accelerator and the resulting plasma cloud is analyzed with suitable instruments. A detailed investigation using latest analyzing techniques like high-speed cameras and sensitive high-resolution spectrometers promises new instrument concepts and insights into short timescale high-pressure states of matter. Linear TOF mass spectrometry provides the opportunity to measure the dynamic and thermodynamic properties of the impact ions. Together with a deeper theoretical understanding of the impact process and the subsequent expansion and other experimental approaches, this method can be a powerful tool to investigate the state of the hot compressed matter due to the related residual ion species.

11:51AM J25.00004 Shock Ejecta Entrapment in Gas, MICHAEL FURNISH, Sandia National Laboratories — In a continuation of earlier work, paired metal shock ejecta experiments, with and without helium fill, are used to measure shock ejecta motion in gas. The vacuum ejecta experiments use Asay foils and PDV to characterize ejecta properties, and the gas ejecta experiments use PDV. FFT analysis of the PDV signals gives a qualitative indication of the presence of such ejecta and of its motion; this can be “calibrated” via the Asay foil data. For modest amounts of ejecta (allowing enough light to reach the free surface and return to the probe to give a strong free surface velocity signal), the FFT amplitudes are roughly proportional to the ejecta areal density, where the proportionality constant depends on the shape and size distribution of the ejecta particles. We assume these are consistent for the two samples in each experiment pair, although limitations to this assumption (e.g. ejecta disruption by the gas) are discussed. An additional caveat is that PDV only measures the motion of ejecta with particle sizes exceeding the 1550 nm light wavelength. Experiments to assess optimal generators of shock ejecta detectable by PDV are also presented. Indium was found to work well in the pressure regime studied.

12:03PM J25.00005 Why nano-projectiles work differently than macro-impactors—role of plastic flow, E.M. BRINGA, CONICET and Instituto de Ciencias Basicas, Universidad Nacional de Cuyo, Mendoza, 5500 Argentina, CHRISTIAN ANDERS, GEROLF ZIEGENHAIN, Fachbereich Physik und Forschungszentrum OPTIMAS, Universitat Kaiserslautern, Germany, GILES GRAHAM, Mineralogy Department, The Natural History Museum, London SW7 5BD, United Kingdom, J. FREDDY HANSEN, Lawrence Livermore National Laboratory, Livermore CA 94550, USA, NIGEL PARK, AWE, Plc Aldermaston, Reading, UK, NICK TESLICH, Lawrence Livermore National Laboratory, Livermore CA 94550, USA, HERBERT URBASSEK, Fachbereich Physik und Forschungszentrum OPTIMAS, Universitat Kaiserslautern, Germany — Hypervelocity impacts provide a way to probe localized regions of a target to extreme pressure and temperature conditions. Retaining crater features can be challenging for hydrocode simulations and test the validity of constitutive models. We will present atomistic simulation data on crater formation due to hypervelocity impact of nanoprojectiles of up to 55 nm diameter and with targets containing up to ten billion atoms, and compare them to available experimental data on micron-, mm-, and cm-sized projectiles. We show that previous scaling laws do not hold in the nano-regime and outline the reasons: within our simulations we observe that the cratering mechanism changes, going from the smallest to the largest simulated scales, from an evaporative regime to a regime where melt and plastic flow dominate, as it is expected in larger micro-scale experiments. The importance of strain-rate dependence of strength and of dislocation production and motion under these extreme conditions will be discussed.

12:15PM J25.00006 Elastic-plastic response and polymorphic phase transition in shock-compressed diamond, YOU LIN, Romain PERRIOT, VASILY ZHAKHOVSKY, Department of Physics, University of South Florida, XIANG GU, Department of Applied Physics, Aalto University, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, Department of Physics, University of South Florida — Shock wave propagation in diamond along the 1 10 2 crystallographic direction was simulated by molecular dynamics (MD) using the reactive empirical bond order (REBO) potential. In addition to known regimes of shock wave propagation, such as single elastic, split elastic-plastic, and single plastic shock wave, two new regimes were observed: 1) a split elastic-plastic shock wave associated with a polymorphic phase transition; 2) a single two-zone elastic-plastic shock wave with the leading elastic zone followed by the plastic zone. In the case of the split elastic-plastic shock wave, the onset of phase transition occurs at a pressure below the Hugoniot elastic limit (HEL); therefore, the solid-solid transformation takes place in the uniaxially compressed material in the absence of plasticity. Within the single two-zone elastic-plastic shock wave, the material in the elastic zone is in a metastable state at a pressure exceeding the HEL. The metastable elastic state decays into the plastic state within the plastic zone, both elastic and plastic fronts moving with the same speed.

**Tuesday, February 28, 2012 11:15AM - 2:15PM**

**Session J25 DCOMP GCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions: Shock Compression and Other High-Strain-Rate Phenomena**

257A
1:03PM J25.00010 Laser-driven focusing shock waves in a thin liquid layer\(^1\), DAVID VEYSSET, THOMAS PEZERIL, GAGAN SAINI, STEVEN KOOI, ALEX MAŽNEV, KEITH NELSON, Massachusetts Institute of Technology — Direct real-time visualization of converging shock waves in a few micron thick liquid layer is demonstrated in an all-optical experiment. The set-up includes an axicon that focuses an intense pico-second excitation pulse into a ring-shaped pattern in a water layer. Optical excitation induces a shock wave that propagates in the plane of the sample and converges toward the center resulting in cylindrical focusing of the shock front. Streak-camera images with a quasi-cw probe beam yield real-time records of the entire shock propagation. Talbot imaging and interferometry with a femtosecond probe pulse are used to obtain full field images at variable delays. Shock pressure values calculated from the velocity of the shock front demonstrate the effect of shock focusing and agree with density profiles obtained by quantitative analysis of interferometric images. The configuration of the experiment provides ample access for optical diagnostics of the shocked material and can be combined with a wide range of spectroscopic probes.

1:15PM J25.00011 From fingering to fracture in a complex fluid, BAUDOUIN SAINTYVES, CEA-Saclay — We present a novel experiment — a specific Hele-Shaw cell with mobile sides which can be pulled at a prescribed velocity - with which both liquids and solids can be loaded with the same boundary conditions, beyond the small deformation regime. With such a system, one can examine quantitatively the response of a viscoelastic material when the loading rate is varied. In the case of viscous Newtonian liquids, an air bubble is shown to destabilize in a Saffman-Taylor manner, forming a finger which elongates in the direction in which the mobile sides are pulled. In contrast, in a Maxwell liquid, we observe a different kind of instability, which gives rise to more complex patterns. This instability leading to local stress concentrations, it is immediately followed by fracture. The displacement field is evaluated in each case by using tracers and image correlations.

1:27PM J25.00012 Nonlinear Elasticity as a Guide for Exploring High Pressure/Shear Stability, T.W. WRIGHT, Johns Hopkins University — Recent constitutive representation theorems for nonlinear anisotropic elasticity, Wright [2011], show the characteristics of elastic response for materials in any point group. All anisotropic representations consist of a sum of six terms, and each term consists of a scalar function of anisotropic invariants times a “tensor generator,” which has the same invariance under group transformations as the stress itself. Knowledge of these representations shows promise as a guide for exploring material stability under extreme loading conditions. Although much is known both experimentally and theoretically about material stability under high pressure, far less is known about the effect of large shear stress superimposed on high pressure. Stress has six independent components, so study of the effects of pressure alone leaves the other five dimensions unexplored. Rather than random DFT calculations in the five dimensional deviatoric space, the known structure of the six term representations suggests that systematic study of just one additional dimension at a time could be accomplished by following changes in just one additional term in the representation at a time. These ideas will be illustrated in the context of a program designed to explore the effect of shear on amorphization in B4C, a ceramic often used for ballistic protection. T.W. Wright, Bootstrap elasticity: From linear to nonlinear constitutive representations, accepted for publication, J. Elasticity.

1:39PM J25.00013 Multi million-to-Billion Atom Molecular Dynamics Simulations of Cavitation-Induced Damage on a Silica Slab, ADARSH SHEKHAR, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, University of Southern California — Cavitation bubble collapse causes severe damage to materials. For example, cavitation erosion is a major threat to the safety of nuclear power plants. The cavitation bubbles may also be utilized for preventing stress corrosion cracking with water jet peening technology. We have performed multi million-to-billion atoms molecular dynamics simulations to investigate the shock-induced cavitation damage mechanism on an amorphous silica slab in water. The system consists of a 60nm thick silica slab immersed in water in an MD box of dimension 265 x 200 x 200 nm\(^3\). A nanobubble is created by removing water molecules within a sphere of radius 100 nm. To apply a planar shock, we assign a uniform particle velocity vp on the entire system towards a planar momentum mirror. We have performed the simulation with two kinds of bubbles, an empty bubble and a bubble filled with inert gas. The simulation results reveal nanojet formation during bubble collapse causing damage on the silica surface; however, the damage was significantly reduced in the case of the filled bubble. We will discuss the effect of the presence of inter gas inside the nanobubble on the pressure distribution, the extent of damage, and collapse behavior corresponding the shock front.
1:51PM J25.00014 Akroleoy: the physics of the extreme behaviour of metals and energetics. NEIL BOURNE, AWE — Structures designed for extreme environments must be designed not only for the magnitude of the load that they will experience, but also the time for which that load acts upon them. At the core of the problem lies the loading impulse experienced by materials and the operating deformation mechanisms that are excited. Our experience of materials’ physics, gathered by investigating response to mechanical loads, has suggested a series of descriptive constructs within which we build our picture of behaviour. At the highest loadings and the shortest loading times this perception is coloured by experience gathered from historical considerations. This paper suggests a framework by which to interpret data collected on the response of metals and explosives. It suggests that strength is a quantity that decays over time and that fundamentally approaches zero in the limit of infinite time. Controlling this decay is the business of engineering to design structures that will survive in the environments our times of interest define.

2:03PM J25.00015 Equation of State of a Solid: Potts-Percolation Model. MIRON KAUFMAN, Cleveland State University, H.T. DIEP, Universite de Cergy-Pontoise, France — We include stress and strain in a Potts-percolation model of a solid, see J. Phys.: Condens. Matter 20, 075222 (2008) and Phys Rev B80, 031116 (2009). Neighboring atoms are connected by a bond of Lennard-Jones energy. If the energy is larger than a threshold the bond is more likely to fail, while if the energy is lower than the threshold the bond is more likely to be alive. We compute the equation of state: stress as function of strain and temperature by using renormalization group and Monte Carlo simulations. The phase diagram and the equation of state are determined. When the Potts heat capacity is divergent the continuous transition is replaced by a weak first-order transition through the van der Waals loop mechanism. When the Potts transition is first order the stress exhibits a large discontinuity as function of the strain.

Tuesday, February 28, 2012 2:30PM - 5:30PM –
Session L25 DCOMP GSCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Warm Dense Matter 257A

2:30PM L25.00001 Simulation of the Correlated Electron Plasma in the Warm Dense Matter Regime by Restricted Path-Integral Molecular Dynamics1. VIVEK KAPILA, University of Florida, PIERRE DEYMIER, University of Arizona, KEITH RUNGE, University of Florida — Warm dense matter (WDM) can be characterized by electron temperatures of a few eV and densities an order of magnitude or more beyond ambient. This regime currently lacks any adequate highly developed class of simulation methods. Recent developments in orbital-free Density Functional Theory (ofDFT) aim to provide such a simulation method, however, little benchmark information is available on temperature and pressure dependence of simple but realistic models in WDM regime. The present work aims to fill this critical gap using the restricted path-integral molecular dynamics (rPIMD) method. Within the discrete path integral representation, electrons are described as harmonic necklaces, while, quantum exchange takes the form of cross linking between electron necklaces. The fermion sign problem is addressed by restricting the density matrix to positive values and a molecular dynamics algorithm is employed to sample phase space. Here, we focus on the behavior of strongly correlated electron plasmas under WDM conditions. We compute the kinetic and potential energies and compare them to those obtained with the ofDFT method.

1Supported in part under US DoE Grant DE-SC0002139.

2:42PM L25.00002 Comparison of Finite Temperature Hartree-Fock and Density Functional Theory for Confined Systems1 , TRAVIS SJOSTROM, S.B. TRICKEY, Quantum Theory Project, University of Florida, FRANK E. HARRIS, Quantum Theory Project, University of Florida and Physics Dept. University of Utah — Warm dense matter (WDM) at elevated temperatures (e.g., T ≈ 1 to several eV) and densities (e.g. one or more orders of magnitude denser than equilibrium) is of growing importance. So far, the most detailed studies of WDM use Born-Oppenheimer molecular dynamics with ground-state density functional theory (DFT) approximations. Little, however, is known about the behavior of the free energy over the temperature and density ranges of interest. In the case of DFT, this deficiency is a barrier to assessing the validity of proposed approximate free-energy functionals. For insight into this problem, we have undertaken systematic numerical study of the thermal Hartree-Fock (THF) approximation. We report progress on application of THF to the problem of eight one-electron atoms at arbitrary positions in a hard-walled box. We discuss the physics which emerges for both high- and low-symmetry ionic arrays, including molecular binding transitions. In addition, we compare the THF results directly with approximate DFT results, including approximate finite-temperature orbital-free kinetic and exchange functionals.

1Supported in part under US DoE Grant DE-SC0002139.

2:54PM L25.00003 The Korringer-Kohn-Rostoker Method Applied to Warm Dense Matter1. DANIEL FINKENSTADT, U.S. Naval Academy, Physics Dept., Annapolis, MD, CHARLES E. NEWNAM, U.S. Naval Academy, Aerospace Dept., Annapolis, MD, BRIAN G. WILSON, Lawrence Livermore National Laboratory, Livermore, CA — The electronic structure, EOS and transport properties of warm electrons in an amorphous or disordered configuration of ions is not well described by either solid-state or plasma models. Such warm, dense systems share the characteristic of the solid state that multi-center scattering effects are of paramount importance in forming bands of valence states. Theoretical treatment of the EOS of warm, dense matter therefore requires a way to include significant occupation of higher energy and angular momentum channel continuum states. We are extending the Green’s function Kohn-Korringer-Rostoker code MECCA as an all-electron (non-pseudo potential) method that treats arbitrary mixtures of atoms on an ab-initio basis over a broad range of conditions, from cold, solid matter up to hot plasmas at extreme (ICF) compression. Specific examples of Aluminum and Boron-Nitride will be discussed.

1Supported by the Military Academy Research Associates program, LLNL/USNA.

3:06PM L25.00004 Density Functional versus Thermal Hartree-Fock Approximations in Warm Dense Lithium1 , VALENTIN V. KARASIEV, TRAVIS SJOSTROM, S.B. TRICKEY, Quantum Theory Project, Physics Dept. U. Florida — We compare the behaviors of the thermal Hartree-Fock (tHF) model and thermal Density Functional Theory (tDFT) using both ground-state and temperature-dependent approximate functionals. The test system is bcc Li in the temperature-density regime of warm dense matter. In the exchange-only case, we find significant qualitative differences between the exact tHF and the DFT calculations with zero-temperature local density approximation (LDA) exchange. A temperature-dependent LDA functional provides much better agreement with the tHF exchange. An underlying need is for well-characterized, reliable pseudopotentials over demanding temperature and density ranges. Thus we compare pseudopotential and all-electron results for small Li clusters of local bcc symmetry and bond-lengths appropriate to high density bulk Li. We determine the density range over which both standard projector-augmented wave (PAW) and norm-conserving pseudopotentials are reliable. Then we construct small-cutoff-radius PAW data sets (for both the local density and the generalized gradient exchange-correlation approximations) which are valid for lithium densities up to at least 80 g/cm³.

1Supported in part under US DoE Grant DE-SC0002139.
3:18PM L25.00005 A Different Time-Dependent Variational Principle Approach: Going Beyond Wave Packet Molecular Dynamics, PAUL GRABOWSKI, Los Alamos National Laboratory, ANDREAS MARKMANN, Yale University, MIKE SURH, Lawrence Livermore National Laboratory, MICHAEL MURILLO, Los Alamos National Laboratory, FRANK GRAZIANI, Lawrence Livermore National Laboratory, CIMARRON COLLABORATION — During inertial confinement fusion, matter evolves from a solid condensed matter phase through the warm dense matter (WDM) regime to a hot dense matter. In WDM, quantum mechanical effects are important because of both Fermi-Dirac statistics and the rate of electrons transitioning in and out of bound states is large. The time-dependent temperature and quickly changing local environment require a time-dependent quantum method. A converged dynamical quantum simulation is intractable for more than a few particles. Instead, we take as a feasible goal to match the statistical properties of a warm dense plasma. The time-dependent variational principle gives a framework for producing equations of motion. A commonly used variational form is a Hartree product of isotropic Gaussian wave packets (wave packet molecular dynamics). The resulting dynamics do not produce the right statistics. We therefore introduce a plane wave basis and discuss its advantages and test its ability to reproduce radial distribution functions produced by hyper-netted chain calculations.

3:30PM L25.00006 All-Electron Path Integral Simulations of Warm, Dense Matter: Application to Water and Carbon, KEVIN DRIVER, Department of Earth and Planetary Science, University of California, Berkeley, USA, BURKHARD MILITZER, Department of Earth and Planetary Science and Department of Astronomy, University of California, Berkeley, CA 94720, USA — We develop an all-electron path integral Monte Carlo (PIMC) method for warm dense matter and apply it to study water and carbon. PIMC pressures, internal energies, and pair-correlation functions compare well with density functional theory molecular dynamics (DFT-MD) at lower temperatures and enable the construction of a coherent equation of state over a density-temperature range of 3–12 g/cm$^3$ and 0–10$^6$ K. PIMC results converge to the Debye-Hückel limiting law at high-temperatures and illuminate the breakdown of DFT pseudopotentials due to core excitations.

3:42PM L25.00007 ABSTRACT WITHDRAWN —

3:54PM L25.00008 Non-equilibrium Warm Dense Matter: Electron-Ion Dynamics of Pumped Nanofoils, YUAN PING, TADASHI OGITSU, ALFREDO CORREA, ERIC SCHWEGLER, GILBERT COLLINS, LLNL, JUN ZHOU, JIANMING CAO, Florida State University, BYOUNG-ICK CHO, KYLE ENGELHORN, PHILIP HEIMANN, ROGER FALCONE, LBNL/UC Berkeley — In 2006, it was reported that the dielectric function of laser-excited gold nanofoils exhibits a peculiar behavior; the interband transition peak of gold is enhanced and undergoes a clear red shift [PRL 96, 255003 (2006)]. In 2009, based on ultrafast electron diffraction measurements on pumped gold nanofoils, it was reported that the time evolution of the Debye-Waller factor is too slow to be explained by a two-temperature model that included temperature dependent el-ph coupling. This anomaly has been attributed to a phonon hardening process caused by high electron temperatures (a few eV) [Science 323, 1033 (2009)]. Later, it was pointed out that at such a high electron temperatures the dielectric function of gold calculated by first-principles DFT simulations does not reproduce the enhanced and red-shifted interband transition peak and an alternative explanation was proposed to reconcile the discrepancies where the effect of ejected electrons was addressed [HEDP 6, 246 (2010)]. In this talk, we will discuss recent experimental/theoretical efforts to further examine the issues relevant to this problem, el-ph coupling, dynamics of ejected electrons, and ballistic transport of electrons [submitted to HEDP; PRL 106, 167601 (2011)].

4:06PM L25.00009 High field terahertz response of materials, DAN DARANCANG, Department of Chemistry, Stanford University, JOHN GOODFELLOW, Department of Materials Science, Stanford University, ALAN FISHER, Linac Coherent Light Source, SLAC National Accelerator Laboratory, AARON LINDENBERG, Department of Materials Science, Stanford University — We report on studies of the response of materials to intense ultrashort electromagnetic fields at terahertz frequencies. These are generated through coherent transition radiation using femtosecond electron bunches at the Linac Coherent Light Source and correspond to single-cycle pulses with electric field amplitudes $\xi$ 20 MV/cm with a frequency centered at 10 THz. Large amplitude nonlinear responses are observed in a range of semiconductor materials associated with field-induced ionization processes, and we show how these processes can be used to carry out nonlinear autocorrelation measurements of the pulse shape. We also discuss recent results probing the response of ferroelectric materials at high fields coupled with ultrafast x-ray probes enabling measurement of their atomic-scale response on sub-picosecond time-scales.

4:18PM L25.00010 An Analytic Screening Potential for Dense, Strongly-Coupled Plasmas, LIAM STANTON, LLNL, MICHAEL MURILLO, LLNL, FRANK GRAZIANI, LLNL — Characterizing warm dense matter (WDM) has gained renewed interest due to advances in powerful lasers and next generation light sources. Because WDM is strongly coupled and moderately degenerate, we must often rely on simulations of WDM, which are necessarily based on molecular dynamics of ions interacting through a screened potential. Almost always, a Debye-Yukawa-like interaction is assumed; however, it is well known that such long wavelength models overscreen. Here, we present a new effective ion-ion interaction, which recovers the exact fermionic linear response in the long-wave limit while retaining a pair-potential functionally similar to that of the Yukawa form. This new potential not only improves the accuracy of screening effects without contributing to the computational complexity of the model, but it also adds physics entirely missing from Yukawa models (such as the onset of Friedel oscillations). Simulations of the ion structure factor are compared to XRTS data for Be and C in the WDM regime.

4:30PM L25.00011 Large-Scale Reactive Simulations of Materials in Extreme Conditions, ANDRES JARAMILLO-BOTERO, WILLIAM GODDARD, California Institute of Technology, MSC TEAM — First-principles quantum mechanics methods are inadequate for accurately describing the effects of thermal, mechanical, chemical or radiation excitations that may occur in materials operating under extreme conditions, or impractical to use due to the prohibitive scaling cost of propagating the total Schrödinger equation for a large set of atoms. In the regime of a high number of electronic excitations, the electronic portion of the wave function contains contributions from many stationary states, and the Born-Oppenheimer approximation breaks down. We have been developing a mixed quantum-classical dynamics approach, called the Electron Force Field (eFF), to simulate the non-adiabatic dynamics of materials in extreme conditions. We have demonstrated its application to describe the: thermodynamics of dense hydrogen over 0-100,000 Kelvin; real-time dynamics of Auger fragmentation of diamond nano particles; transient electronic effects in high-strain rate silicon fracture; Coulomb explosion of carbon clusters; dynamics of cascaded valence ionizations in shocked hydrocarbons; and the dynamics of hypervelocity impact of materials. Here, we summarize our recent progress in the theory and application of eFF for modeling and simulation of materials in extreme conditions.

4:42PM L25.00012 ABSTRACT WITHDRAWN —
4:54PM L25.00013 First-principle Calculations of Equation of State for Metals at High Energy Density. DMITRY MINAKOV, PAVEL LEVASHOV, KONSTANTIN KHISHCHENKO, Joint Institute for High Temperatures RAS — In this work, we present quantum molecular dynamics calculations of the shock Hugoniot of solid and porous samples as well as release isentropes and isentropic sound velocity behind the shock front for aluminum. Also we perform similar calculations for nickel and iron. We use the VASP code with ultrasoft and PAW pseudopotentials and GGA exchange-correlation functional. Up to 512 particles have been used in calculations. To calculate Hugoniot we solve the Hugoniot equation numerically.

To obtain release isentropes, we use Zel dovich's approach and integrate an ordinary differential equation for the temperature thus restoring all thermodynamic parameters. Isentropic sound velocity is calculated by differentiation of pressure along isentropes. The results of our calculations are in good agreement with experimental data at densities both higher and lower than the normal one. Thus, quantum molecular dynamics results can be effectively used for verification or calibration of semiempirical equations of state under conditions of lack of experimental information at high energy densities.

5:06PM L25.00014 Color quantum simulations of strongly coupled quark-gluon plasma. VLADIMIR FILINOVIĆ, VLADIMIR FORTOV, Joint Institute for High Temperatures RAS, Moscow, Russia, MISHAEL BONITZ, Institute for Theoretical Physics and Astrophysics, Kiel, Germany, YURI IVANOV, GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany, PAVEL LEVASHOV, Joint Institute for High Temperatures RAS, Moscow, Russia — We propose stochastic simulation of thermodynamics and kinetic properties for quark-gluon plasma (QGP) in semi-classical approximation in the wide region of temperature, density and quasi-particles masses. In grand canonical ensemble for finite and zero baryon chemical potential we use the direct quantum path integral Monte Carlo method (PIMC) developed for finite temperature within Feynman formulation of quantum mechanics to do calculations of internal energy, pressure and pair correlation functions. The QGP quasi-particles representing dressed quarks, antiquarks and gluons interact via color quantum Keldysh pseudopotential rigorously derived for Coulomb particles. This method has been successfully applied to strongly coupled electrodynamic plasmas (EMP). A strongly correlated behavior of the QGP is expected to show up in long-ranged spatial correlations of quarks and gluons which, in fact, may give rise to liquid-like and, possibly, solid-like structures. We have done already the first calculation of the QGP equation of state, spatial and color pair distribution functions, diffusion coefficients and shear viscosity.

5:18PM L25.00015 Proton crystallization and quantum melting of proton crystals in a dense hydrogen plasma. PAVEL LEVASHOV, VLADIMIR FORTOV, VLADIMIR FILINOVIĆ, Joint Institute for High Temperatures RAS, Moscow, Russia, HOLGER FEHSE, Institut fur Physik, EMAU Greifswald, Germany, MICHAEL BONITZ, Institute for Theoretical Physics and Astrophysics, Kiel University, — We present extensive new simulation results which allow to predict the temperature and density range for proton crystallization. We simulate a macroscopic spatially homogeneous fully ionized two-component electron-proton plasma in thermodynamic equilibrium from first principles using direct fermionic path integral Monte Carlo simulations. Our results for the phase diagram differ substantially from the previous predictions based on the one-component plasma (OCP) model: In the classical part of the phase diagram the crystal appears to be stabilized compared to the OCP prediction. In contrast, in the quantum part of the phase diagram the crystal appears to be de-stabilized and vanishes at lower densities compared to the OCP prediction. Finally, the maximum temperature for the proton crystal is found to be around 40 000K, slightly below the previous prediction. Our results indicate that the OCP treatment of the liquid-solid transition in a two-component plasma has to be questioned. The OCP-assumption of a homogeneous rigid neutralizing background gives rise to substantial deviations of the critical parameters.

Tuesday, February 28, 2012 5:45PM - 6:45PM — Session M25 GSCCM: GSCCM Business Meeting 257A

5:45PM M25.00001 GSCCM Business Meeting —

Wednesday, February 29, 2012 8:00AM - 11:00AM — Session P25 DCOMP GSCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Static Pressure 257A

8:00AM P25.00001 A new metastable phase of silicon in the Ibam structure. BRAD D. MALONE, MARVIN L. COHEN, Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory — In a study aimed at finding new useful forms of silicon, we use an ab initio random structure searching (AIRSS) method to identify a new phase of silicon in the Ibam structure. The Ibam phase is found to be semimetallic within density functional theory with a small band overlap, and it is expected that quasiparticle corrections using the GW approximation would yield a semiconducting state with a small band gap. Calculation of the lattice dynamics reveals that the structure is locally stable. Enthalpy-pressure relations are calculated for the Ibam structure as well as all other known Si structures, including the previously predicted phases st12 and bct. These results indicate that Ibam silicon is metastable over the pressure range considered. Calculated coexistence pressures of the other known phase transitions are in good agreement with experimental observation.

8:12AM P25.00002 Ultra-incompressible Three Dimensional Long-range Ordered Amorphous Carbon Clusters1. LIN WANG, Carnegie Institution of Washington, 1HPSYNC, GEOPHYSICAL LABORATORY, CARNEGIE INSTITUTION OF WASHINGTON, ARGONNE, IL 60439, USA TEAM — Here we report the synthesis of a long range ordered material constructed from units of amorphous carbon clusters and solvent molecules. This material has super-incompressibility which can make indents on diamonds. It was synthesized by crushing the fullerenes cages at high pressure. Using high pressure x-ray diffraction and Raman spectroscopy, we observed that the fullerenes cages collapse as the pressure higher but the sample remains in crystalline phase even at 60 GPa. The high pressure phase is ultra-incompressible, quenchable and much denser than the starting material. The discovery of the existence of such a unique phase should lead to a great deal of interest for design and synthesis of materials with this characteristic.

1This work was supported as part of the EFRee, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science under Award Number DE-SC0001057.

8:24AM P25.00003 Anharmonicity and bonding electrons in silicon under high pressures. GUOYIN SHEN, DAJO IKUTA, HPCAT, Carnegie Institution of Washington — Electron density distributions have been measured for silicon at high pressures by single crystal diffraction using a diamond anvil cell. An abrupt change in charge density distribution is observed at 10.1 GPa, a pressure close to a phase transition from diamond structure to beta-tin structure at 12.5 GPa. Our results show a strong anharmonicity effect in silicon in a pressure range of 2.5 GPa before the phase transition to beta-tin.
8:36AM P25.00004 Formation of superconducting platinum hydride under pressure: an ab initio approach. DUCK YOUNG KIM, Geophysical laboratory, Carnegie institution of Washington. RALPH SCHEICHER, Uppsala University, Uppsala, Sweden, CHRIS PICKARD, University College London, London, UK, RICHARD NEEDS, University of Cambridge, Cambridge, UK, RAJEEV AHuja, Uppsala University, Uppsala, Sweden — Noble metals such as Pt, Au, or Re are commonly used for electrodes and gaskets in diamond anvil cells for high-pressure research because they are expected to rarely undergo structural transformation and possess simple equation of states. Specifically Pt has been used widely for high-pressure experiments and has been considered to resist hydride formation under pressure. Pressure-induced reactions of metals with hydrogen are in fact quite likely because hydrogen atoms can occupy interstitial positions in the metal lattice, which can lead to unexpected effects in experiments. In our study, PRL 107 117002 (2011), we investigated crystal structures using ab initio random structure searching (AIRSS) and predicted the formation of platinum mono-hydride above 22 GPa and superconductivity Tc was estimated to be 10 – 25 K above around 80 GPa. Furthermore, we showed that the formation of fcc noble metal hydrides under pressure is common and examined the possibility of superconductivity in these materials.

8:48AM P25.00005 New ultrahigh pressure phases of H2O ice predicted using an adaptive genetic algorithm1. MIN JI, CAI-ZHUANG WANG, Iowa State University, KOICHIRO UMEmOTO, University of Minnesota, KAI-MING HO, Iowa State University, RENATA WENTZCOVITCH, University of Minnesota — We propose three new phases of H2O under ultrahigh pressure. Our structural search was performed using an adaptive genetic algorithm which allows an extensive exploration of crystal structure at density functional theory(DFT) accuracy. The new sequence of pressure-induced transitions beyond ice X at 0 K should be ice X → Pbcn → Pm1c2 → Pm1c2 → F21 → P21/c phases. Across the Pm1c2 → P21 transition, the coordination number of oxygen increases from 4 to 5 with a significant increase of density. All stable crystalline phases have nonmetallic band structures up to 7 TPa.

3MJ,CZW, and KMH were supported by the US Department of Energy, Basic Energy Sciences, Division of Materials Science and Engineering, under Contract No. DE-AC02-07CH11358. KU and RMW were supported by EAR-0757903, 0810272, 1047629, and ATM-0426757 (YLab).

9:00AM P25.00006 Quantum Monte Carlo applied to Solids under Pressure, LUKE SHULENBURGER, T.R. MATTSSON, Sandia National Laboratories — Diffusion quantum Monte Carlo (DMC) has been applied to solids under pressure in several different contexts a high degree of success1. All of these calculations must address three errors present in DMC calculations of solids: the fixed node approximation, the pseudopotential approximation and the finite size approximation. Due to the varying approximations to address these errors, these calculations suffer from an uncertainty that is almost comparable to that introduced by the choice of functional in density functional theory (DFT). In this presentation, we present lattice constants and bulk moduli of more than fifteen solids under compression performed with a consistent approach to these three approximations. These results help establish the general accuracy that may be expected from DMC calculations of solids under pressure and also provide a reference from which improvements to DMC methods may be judged. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

9:12AM P25.00007 First-principles simulations on bonding pathways of chemical transformations under hydrostatic compression. ANGUANG HU, FAN ZHANG, DRDC Suffield — High pressure as a thermodynamic parameter provides a strong structural constraint to lead chemical transformations with selective ways. Thus, chemical transformations under pressure can create novel materials which may not be accessible by covalent synthesis. However, bonding evolution toward high pressure chemical transformations can be a complex process and may happen over widely different pressures. To understand bonding evolution pathways of high pressure chemical transformations, first-principles simulations were performed following hydrostatic compression enthalpy minimization paths to obtain experimentally and theoretically established phase transitions of carbon. The results showed that the chemical transformations from hydrostatic compression carbon to single-bonded phases were characterized by a sudden decrease in principal stress components, indicating the onset of chemical transformation. On this basis, a number of hydrostatic compression chemical transformations from molecular precursors to novel materials were predicted, such as hydrocarbon graphene, a hydrogenated carbon nitride sheet, and carbon nitrides. All predicted hydrostatic compression transformations are featured as a sudden change in principal stress components, representing chemical bonding destruction and formation reactions with a cell volume collapse.

9:24AM P25.00008 Dielectric constant of water under deep Earth pressures and temperature conditions1. DING PAN, LEONARDO SPANU, Department of Chemistry, University of California, Davis, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry, University of California, Davis, Department of Physics, University of California, Davis — The knowledge of the dielectric constant of water as a function of pressure (P) and temperature (T) plays a critical role in understanding the chemistry of aqueous systems, and in particular of fluids in the Earth mantle, where water is stored in hydrous minerals. By using first-principles molecular dynamics, we have computed the dielectric constant of water at T = 1000 K, between 1 and 10 GPa, under conditions of the Earth upper mantle. We present a detailed comparison of our results with available experimental data and empirical models, and we discuss how the liquid dielectric constant is affected by the changes in the hydrogen-bond network and molecular dipole moment observed upon compression.

9:36AM P25.00009 Hydrogen-Helium Mixtures at High Pressures. MIGUEL A. MORALES, SEBASTIEN HAMEL, KYLE CASPERSEN, ERIC SCHWEGLER, LLNL — We extend our previous work on hydrogen-helium mixtures (Morales, M. A., et. al. PNAs 106, 1324 (2009)). Many pressures and lower temperatures, across the molecular dissociation regime in hydrogen, to the low pressure molecular liquid. Using density functional theory-based molecular dynamics together with thermodynamic integration techniques, we calculate the Gibbs free energy of the dense liquid as a function of pressure, temperature, and composition. Our work focuses on the mixing properties of the liquid, the optical properties including conductivity and reflectivity, and the creation of accurate mixing models for thermodynamic properties, including pressure and entropy. The resulting models will provide the basis for accurate first-principles equations of state for planetary modeling. Prepared by LLNL under Contract DE-AC52-07NA27344.

9:48AM P25.00010 Pressure makes mercury a transition metal: a first-principles study of HgF4 solid phases. XIAOLI WANG, HAIQING LIN, Beijing Computational Science Research Center, YANMING MA, State Key Lab of Superhard Materials, Jilin University, MAOSHENG MIAO, Materials Research Lab, University of California, Santa Barbara — Mercury is considered as a post-transition metal, because its d shell is filled and does not involve in forming chemical bonds. Yet, because the large relativistic effect pushes up the outmost d level, there is a high expectation that Hg can be stabilized in a higher oxidation state. The HgF4 molecule has been predicted by calculations, and an evidence of such molecule is shown by IR absorption recently. However, there is neither computation nor experiment report on possible high oxidation state of Hg in solid. By using first-principles density functional theory and a structure-searching method, we studied the structural change of a solid system of Hg and F under pressures from 0 to 300 GPa. We found that at lower pressure, the stable structure consists of F2P2 and F2 molecules. At about 25 GPa, the system undergoes a structural change and forms HgF4 planar molecules featuring d8 configuration. The calculations show that the d orbitals of Hg involve in chemical bonding, which is the signature of a transition metal.
The presence of aluminum, however, does affect the population of ferric iron significantly – the majority of \( \text{Fe}^{3+} \) overall phase stability of the mixture under conditions relevant to the planetary interiors.

We present results concerning the computational study of the physical properties of a fluid compositionally similar to what is expected in the interior of Uranus and Neptune. Our diffusivity and non-axial magnetic fields of these planets originate from a thin convective and conducting shell of material around a stratified fluid core. We present a computational study of the fluid compositionally similar to what is expected in the interior of Uranus and Neptune represent important observables for constraining and developing deep interior models. Models suggest that the non-dipolar and configuration of aluminum.

This work was supported by the MRSEC Program of NSF grants DMR 0212302 and DMR-0819885. Calculations were performed at the Minnesota Supercomputing Institute (MSI).

10:36AM P25.00014 Effects of aluminum on spin-state crossover of iron in the Earth’s lower mantle \(^1\), RENATA WENTZCOVITCH, HAN HSU, YONGGANG YU, University of Minnesota — Using density functional theory + Hubbard \( U \) (DFT+\( U \)) calculations, we investigate how aluminum affects the spin states of iron in magnesium perovskite and post-perovskite, the major mineral phases in and at the bottom of the Earth’s lower mantle. We find that aluminum does not change the response of iron spin state to the increasing pressure, namely, only the ferric iron \( \text{Fe}^{3+} \) residing the octahedral (B) site undergoes a crossover from high-spin to low-spin state, same as aluminum-free iron-bearing magnesium silicate \( (\text{MgSiO}_3) \) perovskite and post-perovskite (Ppv), a major mineral phase in the Earth’s D’ layer, where the pressure ranges from about 120 to 135 GPa. In this pressure range, ferrous iron \( \text{Fe}^{2+} \) substituting for manganese at the dodecahedral (A) site remains in the high-spin (HS) state; intermediate-spin (IS) and low-spin (LS) states are highly unfavorable. As to ferric iron \( \text{Fe}^{3+} \), which substitutes magnesium at the A site and silicon at the octahedral (B) site to form \( (\text{Mg,Fe})(\text{Si,Fe})\text{O}_3 \) Ppv, we find the combination of HS \( \text{Fe}^{3+} \) at the A site and LS \( \text{Fe}^{3+} \) at the B site the most favorable. Neither A-site nor B-site \( \text{Fe}^{3+} \) undergoes a spin-state crossover in the D’ pressure range. The computed iron quadrupole splittings are consistent with those observed in Mössbauer spectra. The effects of \( \text{Fe}^{2+} \) and \( \text{Fe}^{3+} \) on the equation of state of Ppv are found nearly identical, expanding the unit cell volume while barely affecting the bulk modulus.

This work was supported by the MRSEC Program of NSF grants DMR 0212302, DMR-0819885, EAR-081272, and EAR-1047629. Calculations were performed at the Minnesota Supercomputing Institute (MSI).

10:48AM P25.00015 Phase stability of mixtures at extreme conditions: implications for the interior structure of the Outer Planets, SEBASTIEN HAMEL, Lawrence Livermore National Lab — The unusual magnetic fields of the planets Uranus and Neptune represent important observables for constraining and developing deep interior models. Models suggest that the non-dipolar and non-axial magnetic fields of these planets originate from a thin convective and conducting shell of material around a stratified fluid core. We present a computational study of the physical properties of a fluid compositionally similar to what is expected in the interior of Uranus and Neptune. Our diffusivity and conductivity results suggest that the core cannot be well mixed if it is to generate non-axisymmetric magnetic fields. The simulations highlight the importance of chemistry on the properties of this complex mixture, including the possible formation of carbon and nitrogen clusters. We present results concerning the overall phase stability of the mixture under conditions relevant to the planetary interiors.

Wednesday, February 29, 2012 11:15AM - 2:03PM –
Session Q25 DCOMP GCCCM DMP: Focus Session: Simulation of Matter at Extreme Conditions - Phase Transitions

11:15AM Q25.00001 Metallization of FeO at High Temperatures and Pressures: DFT-DMFT Computations and Comparisons with Experiments, R.E. COHEN, Geophysical Laboratory, Carnegie Institution, KRISTJAN HAULE, Dept. Physics, Rutgers University — DFT+Dynamical Mean Field Theory (DMFT) was applied to FeO as a function of pressure and temperature. We use an LAPW basis set, and the lattice terms are evaluated using the WIEN2K LAPW code. The impurity model is solved using continuous time quantum Monte Carlo (CTQMC). Temperature enters explicitly, so we made special efforts to understand high temperature behavior. The calculations are fully self-consistent, including the impurity levels and crystal field splitting, and the total energy is evaluated using the full potential and charge density of the lattice plus impurity models. We find with increasing pressure in paramagnetic FeO in a cubic lattice and \( U = 0 \) eV a high-spin low-spin transition, with a wide transition region between characterized by intermediate occupancies of the t2g and eg states between. We find that at 300K cubic FeO remains insulating to a factor of two compression (over 600 GPa), except for a small region of high spin metal. However, at high temperatures (e.g. 2000K) a metallic state is found. We find excellent agreement with recent high temperature high pressure experiments (Ohta et al.). We are now studying the antiferromagnetic ordering and effects of lattice strain.

11:27AM Q25.00002 ABSTRACT WITHDRAWN
11:39AM Q25.00003 Finite-temperature solid phases and melting of denser lithium\(^1\). Sabri Elatresh, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada; Stanimir Bonev, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada; Lawrence Livermore National Laboratory, Livermore, California 94550 — There has been a lot of recent interest in lithium at high pressure, in particular, in relation to deviations from simple metallic behavior, non-intuitive structural changes, and its anomalous melting curve. Most of the theoretical studies have been limited to 0 K static lattices and liquid properties with classical ions. In this talk, we will present results for the stability of lithium up to 250 GPa and finite temperature, as well as its melting curve. Comparison with experimental observations and the significance of quantum ion dynamics for the measured properties will be discussed.

\(^1\)Work supported by NSERC, Acenet, and LLNL under Contract DE-AC52-07NA27344.

11:51AM Q25.00004 Study on the release process of \(\gamma\) and \(\alpha\) phase transition in cerium material\(^1\). Xiaomin Hu, Hao Pan, National Key Lab of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, China; Chengda Dai, Qiang Wu, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang 621900, China; National Key Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, China; Laboratoire de Physique des Matériaux, Université de Lyon, France — Cerium has lots of phase transition in high pressure and temperature. A volume change of about 15% occurs when Cerium is subject to high pressure (~0.7GPa) and \(\gamma\) \(\rightarrow\) \(\alpha\) phase change takes place. The phase transition and constitutive model of Cerium can be respectively obtained by calculating the experiment results and taking account of the multi-phase equation of state (EOS). The calculated results indicate that in loading condition the phase transition pressure of Cerium is higher than quasi-static compression. The calculated results indicate that the phase transformation under release is difficult described because the \(\alpha\) \(\rightarrow\) \(\gamma\) phase reversal is great influenced by plastic flow. Based on multi-phase equation of state, constitutive model and non-equilibrium phase transition equation, introducing quasi-elastic-unloading rate simulated the phase transition under release. The calculated result is according with the experiment.

\(^1\)Work supported by NSERC, LLNL, CFI, and Killam Trusts. Prepared by LLNL under Contract DE-AC52-07NA27344.

12:03PM Q25.00005 Stability of dense liquid carbon dioxide\(^1\). Brian Boates, Lawrence Livermore National Laboratory, Dalhousie University, Amanuel Teveldeberhan, Lawrence Livermore National Laboratory, Stanimir Bonev, Lawrence Livermore National Laboratory, Dalhousie University — We have used first-principles molecular dynamics to identify a transition from molecular liquid CO\(_2\) to a new polymeric liquid phase under compression. The phase transition is first-order and unlike other such transitions, is not accompanied by metalization. The region near the liquid-liquid-solid triple point is particularly interesting as it coincides with pressure-temperature conditions inside the Earth’s mantle. We have characterized the stability of CO\(_2\) under these conditions; contrary to previous studies, our calculations show that CO\(_2\) does not phase separate into carbon and oxygen. Comparisons with and alternative interpretations of previous measurements will be presented. Routes for experimental detection of our predictions will also be discussed.

\(^1\)Work supported by US DOE’s Energy, Basic Energy Sciences, Division of Materials Science and Engineering, under Contract No. DE-AC02-07CH11358. Ku and RMW was supported by NSF grants ATM-0426757 (VLab) and EAR-1047629.
12:51PM Q25.00009 Raman study of the Verwey transition in Magnetite at high-pressure and low-temperature; effect of Al doping¹, LEV GASPAROV, Z. SHIRSHIKOVA, T.M. PEKAREK, J. BLACKBURN, Department of Physics, University of North Florida, Jacksonville, V. STRUZHKIN, A. GAVRILIUK², Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C., R. RUECKAMP, University of Cologne, Institute of Physics 2, Cologne, Germany, H. BERGER, Ecole Polytechnique Federale de Lausanne, Switzerland — We report high-pressure low-temperature Raman measurements of the Verwey transition in pure and Al –doped magnetite (Fe₃O₄). Al-doped magnetite Fe₂,₈Al₀,₂O₄ (Tᵥ=116.5K) displays a nearly linear decrease of the transition temperature with an increase of pressure yielding dP/dTᵥ=-0.096±0.013 GPA/K. In contrast pure magnetite displays a significantly steeper slope of the PT equilibrium line with dP/dTᵥ = -0.18±0.013 GPA/K. Contrary to earlier high pressure resistivity reports we do not observe quantum critical point behavior at 8 GPa in the pure magnetite. Our data indicates that Al doping leads to a smaller entropy change and larger volume expansion at the transition. The trends displayed by the data are consistent with the mean field model of the transition that assumes charge ordering in magnetite.

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²Russian Academy of Sciences Institute for High Pressure Physics, Troitsk, and Institute of Crystallography, Moscow.

1:03PM Q25.00010 Magnetic and Thermal Fluctuations in Fe and (Fe,Ni) alloys at Earth Core Conditions¹, SUFIAN ALNEMRAT, BORIS KIEFER, New Mexico State University — Several lines of evidence suggest that the earth’s inner core is dominated by an iron rich (Fe,Ni) alloy. In this study we address the influence of magnetic and thermal fluctuations as driving forces for phase transitions in Fe and FeNi structures at inner core pressure and temperature conditions. Bcc iron is stable at ambient conditions due to its ferromagnetic nature which highlights the importance of magnetism for structural stability. Ab-initio electronic structure calculations are used to study the thermal and magnetic fluctuations in Fe and (Fe,Ni) alloys up to pressures and temperatures expected in the earth’s inner core. The variable cell shape molecular-dynamics simulations include the magnetic moment and thermal fluctuations. Our preliminary results show a phase transformation in hcp-Fe-Ni alloy that occurs after 2.5 ps, well after equilibration. The correlation of magnetic and thermal fluctuations suggests that the residual magnetism is too weak to induce the observed transition. Instead, large thermal fluctuations at the onset of the transition provide a likely driving force.

¹The authors gratefully acknowledge funding from NSF through grant EAR-0636075.

1:15PM Q25.00011 Mechanism of body-centered cubic phase stabilization in Fe and He at high pressure and temperature, ANATOLY BELONOSHKO, KTH Royal Institute of Technology, Stockholm, Sweden, SERGIU ARAPAN, Uppsala University, Uppsala, Sweden, LOVE KOCI, AWA Patent AB, Stockholm, Sweden, ANDERS ROSENGREN, KTH Royal Institute of Technology, Stockholm, Sweden — We have investigated the stabilization of the body-centered cubic phase in Fe and He at high P and T by means of ab initio and classical molecular dynamics. These phases are dynamically unstable at high P and low T, however, they become dynamically stable at high T. We calculated the phonon density of states for Fe and He phases and observed that the bcc PDOS contains long-wavelength phonon states (absent in the close packed phases) that contribute to the free energy. This observation is consistent with the mechanism of stabilization proposed earlier (P. Loubeyre, J.-P. Hansen, PRB 31, 634 (1985); B. L. Holian et al., JCP 59, 5444 (1973)). Direct ab initio simulations of Fe crystallization and classical co-existence simulations for He indicate that the bcc phase is a submelting phase at high P. Previous calculations of the free energy in the bcc phase have been performed on small samples and could not adequately take the long-wavelength correlated motion into account.

1:27PM Q25.00012 ABSTRACT WITHDRAWN —

1:39PM Q25.00013 Computation of free energy of liquids and its application to melting of CO₂ and N², AMANUEL TEWELDEBRHAN, Lawrence Livermore National Lab, BRIAN BOATES, STANIMIR BONEV, Dalhousie University and Lawrence Livermore National Lab — A computationally efficient method is proposed to compute the free energy of liquids with accuracy comparable to ab initio thermodynamic integration. The method has been applied to predict melting curves of CO₂ and N₂ over a wide range of pressure using the solid-liquid phase coexistence approach. The calculated melting lines are compared with available experimental data and the crossing of the geotherm and melting line of CO₂ is determined.

²Work supported by LLNL, ACEnet, NSERC, and CFI. Prepared by LLNL under Contract DE-AC52-07NA27344.

1:51PM Q25.00014 Melting behaviour of high pressure Na. An ab initio study, DAVID J. GONZALEZ, Dpt Fisica Teorica, Universidad de Valladolid, Valladolid, LUIS E. GONZALEZ, Dpt Fisica Teorica, Universidad de Valladolid, Valladolid — The melting curve of sodium for a pressure range up to 120 GPa has been evaluated by the orbital free ab initio molecular dynamics method. This method uses the electronic density as the basic variable and scales almost linearly with system size which allows to perform simulations with a large number of particles and for long simulation times. For various pressures and temperatures we have calculated some static properties (pair distribution functions, static structure factors and short-range order parameters), dynamic properties (mean square displacement, velocity autocorrelation functions and dynamic structure factors) and transport coefficients (self-diffusion, adiabatic sound velocities and shear viscosities). The calculated melting curve reproduces the main qualitative features found in the experiment.