WDM2019

10th International Workshop on Warm-Dense-Matter 2019

Scientific Schedule

Monday, 6th May 2019

Session 1	
09:00	Welcome *T. Tschentscher (EUXFEL), B. Ziaja-Motyka (DESY)*
09:10	**Structural dynamics of ultrafast laser-excited copper** *MO, Mianzhen (SLAC national accelerator laboratory)*
09:40	**Electron kinetics induced by ultrafast photo-excitation** *NG, Andrew(Department of Physics & Astronomy, University of British Columbia, Canada)*
10:00	**X-ray absorption spectroscopy with a laser-produced betatron source** *LECHERBOURG, Ludovic (CEA)*
10:20	**Simulating the ultrafast nonequilibrium electron dynamics in warm dense matter** *BONITZ, Michael (Uni Kiel)*
10:40	**Study of Mixtures Across the Warm-Dense-Matter Regime** *TICKNOR, Christopher (Los Alamos National Laboratory)*
11:00	***Coffee break***
Session 2	
11:30	**Development of Finite-Temperature Exchange-Correlation Functionals: Improving Reliability for Warm-Dense-Matter Applications** *KARASIEV, Valentin (Laboratory for Laser Energetics, University of Rochester)*
12:00	**Ab Initio Path Integral Monte Carlo Results for the Dynamic Structure Factor of Correlated Electrons: From the Electron Liquid to Warm Dense Matter** *DORNHEIM, Tobias (Kiel University)*
12:20	**Thermodynamics of Shock and Isentropic Compression of Warm Dense Matter** *FORTOV, Vladimir E. (Joint Institute for High Temperatures of RAS)*
12:40	**The High-Pressure Melting Line and Band-Gap Closure in Helium** *PREISING, Martin (University of Rostock)*
13:00	***Lunch break***
Session 3	
14:30	**Polymorphism, amorphization and melting of shocked MgSiO3 from in situ X-ray diffraction** *HERNANDEZ, Jean-Alexis (Laboratoire d'Utilisation des Lasers Intenses, Ecole Polytechnique)*
15:00	**Properties of water under ultrahigh pressure by combining DAC static and high power laser dynamic loading** *HUANG, Xiuguang (Shanghai Institute of Laser Plasma)*
15:20	**Sound velocity of quasi-isentropic compressed dense deuterium up to Mbar pressure** *YUNJUN, Gu (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China)*

15:40	**Ab initio study of Iron-Nickel alloys in Super-Earths cores** *SOUBIRAN, François (ENS Lyon)*
16:00	***Coffee break***
Session 4	
16:30	**Non-equilibrium electron kinetics in warm dense Au** *WANG, Xiaowei (1Department of Physics, National University of Defense Technology, China)*
17:00	**Ab initio calculation of electron impact ionization for ions in exotic electronic configurations** *BEKX, John Jasper (CFEL/DESY)*
17:20	**Dynamics and Properties of High-Density Surface Plasmas Induced by Cold X-rays** *MILOSHEVSKY, Gennady (Virginia Commonwealth University)*
17:40	**Surface dynamics of solids upon high-intensity laser irradiation investigated by grazing incidence X-ray surface scattering** *NAKATSUTSUMI, Motoaki (European XFEL)*
18:00	**End of Day 1**

Tuesday, 7th May 2019

Session 5	
09:00	**Measuring Plasma Parameters of Warm Dense Matter from X-Ray Thomson Scattering at the LCLS and the NIF** *REDMER, Ronald (Universität Rostock)*
09:30	**Characterising the icy giant planets' interiors via laser-driven shock compression of water, ammonia, and a C:H:N:O mixture** *GUARGUAGLINI, Marco (Laboratoire LULI, École Polytechnique)*
10:00	**Thermodynamic properties of C-N-O-H mixture in the region of non-ideal plasma** *RYKOUNOV, Alexey (Russian Federal Nuclear Center – Academician*
10:20	**Multiple shock reverberation compression of dense Ne up to warm dense regime: evaluating the theoretical models** *TANG, Jun (Science and Technology on Surface Physics and Chemistry Laboratory)*
10.40	**Observation of Nonlocal Electron Transport in Warm Dense CH** *FALK, Katerina (Helmholtz-Zentrum Dresden-Rossendorf)*
11:00	***Coffee break***
Session 6	
11:30	**Using intense laser-driven proton beams to produce warm, dense materials** *McGUFFEY, Chris (University of California San Diego)*
12:00	**Electronic Transport Properties of Warm Dense Matter from Time-dependent Density Functional Theory** *CANGI, Attila (Sandia National Laboratories)*
12:30	**A theoretical simulation for nonequilibriumelectronic kinetics of warm dense gold** *GAO, Cheng (National University of Defense Technology)*
12:50	**Electron-ion coupled dynamics of warm dense matter** *DAI, Jiayu (National University of Defense Technology)*
13:10	***Lunch***
Session 7	
14:30	**Time-resolved Electrical Conductivity of Warm Dense Gold Measured by Multi-cycle THz**

	Radiation *CHEN, Zhijiang (SLAC National Accelerator Laboratory)*
15:00	**Dynamic Band Occupation and Optical Response of Warm Dense Gold** *NDIONE, Pascal*
15:20	**Effect of an harmonicity on the hcp to bcc transition in beryllium at high pressure and high temperature conditions** *SONG, Haifeng (IAPCM)*
15:40	**Kinetics and structural changes in shock-compressed bismuth** *PÉPIN, Charles (CEA)*
16:00	***Coffee break***
16:30	**Poster session**
18:00	**End of day 2**

Wednesday, 8th May 2019

Session 8	
09:00	**Recent experimental investigations of deuterium at warm dense matter conditions** *CELLIERS, Peter M. (Lawrence Livermore National Laboratory)*
09:30	**The classical molecular dynamics at the service of experiments** *SOULARD, Laurent (CEA, DAM, DIF)*
10:00	**Femtosecond laser-produced periodic plasma in a colloidal crystal probed by XFEL radiation** *MUKHARAMOVA, Nastasia (DESY)*
10:20	**X-ray diffraction of warm dense matter on the Z-accelerator** *AO, Tommy (Sandia National Laboratories)*
10:40	**Dynamics of the Electrical Conductivity and Structure of Warm Dense Aluminum Studied by Single - Shot Terahertz Spectroscopy and Ultrafast Electron Diffraction** *OFORI-OKAI, Benjamin K. (SLAC)*
11:00	**Coffee break**
11:30	**Special session**
13:00	***Lunch***
Session 9	
14:30	**Electron kinetics induced by X-ray FEL excitation of Au** *ZIAJA, Beata (CFEL,DESY)*
15:00	**Emission wavelength control in hard x-ray lasers with Bragg crystal target** YONEDA, Hitoki (Institute for Laser Science)
15:20	**Ultrafast Anisotropic Disordering in X-ray Heated Graphite** *HARTLEY, Nicholas (HZDR)*
15:40	**Energy relaxation and electron phonon coupling in laser heated solids** *VORBERGER, Jan (HZDR)*
16:00	***Coffee break***

Session 10	
16:30	**Development of the National Ignition Facility ramp compression platform and the use of ramp compression experiments in construction of material models** *ALI, Suzanne*
17:00	**Paramagnetic-to-diamagnetic transition in dense liquid iron and its influence on electronic transport properties** *FRENCH, Martin (Universität Rostock)*
17:20	**Charged Particle Stopping Power of Nonideal Plasmas** *GERICKE, Dirk (University of Warwick)*
17:40	**Characterizing the Ionization Potential Depression in Dense Carbon Plasmas with High-Precision Spectrally Resolved X-ray Scattering** *KRAUS, Dominik (HZDR)*
18:00	**End of conference**

Structural dynamics of ultrafast laser-excited copper

Here we report the structural dynamics study of ultrafast laser-excited copper using the technique of time-resolved electron diffraction. In our experiments, 40-nm-thick polycrystalline copper films were irradiated by 400nm, 130fs (FWHM) laser pulses to produce isochoric heated warm dense states. Structural evolution of the excited target as it underwent solid-liquid phase transition was studied with electron diffraction at relativistic energies to provide atomic resolution of the nuclear response. We observed homogeneous melting that occurs below 20ps at absorbed energy densities of ˜1.2-2.5MJ/kg. The measured decay of Laue diffraction peak intensities in the first 5ps were employedto calculate the ion temperature change in the early time when no significant lattice expansion isexpected. Furthermore, the liquid structure factor data to large wavenumbers allows us to inferthe ion temperature at the melt time by comparing with DFT-MD simulations. These inferred ion temperature results were understood with TTM simulations, suggesting an electron-ion coupling strength significantly lower than the temperature-dependent value calculated by density functional theory [1].

[1] Z. Lin, et al., Phys. Rev. B 77, 075133 (2008).

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Primary author(s) : Dr. MO, Mianzhen (SLAC national accelerator laboratory)
Co-author(s) : Dr. OFORI-OKAI, Benjamin (SLAC National Accelerator Laboratory);Dr. WITTE,Bastian, Bernhard, Lothar (Rostock University, SLAC);Mr. SCHORNER, Maximillian (Universität Rostock);Dr. SHEN, Xiaozhe (SLAC);Dr. CHEN, Zhijiang (SLAC National Accelerator Laboratory);Mrs. BECKER, Valerie (Southern Illinois University Edwardsville);Dr. DUNNING, Michael(SLAC);Dr. LI, Renkai (SLAC);Dr. WEATHERSBY, Stephen (SLAC);Prof. REDMER, Ronald(Universität Rostock);Dr. WANG, Xijie (SLAC);Prof. GLENZER, Siegfried (SLAC)

Electron kinetics induced by ultrafast photo-excitation

We report on the measurement of the temporal evolution of ac conductivity and electron density resulting from fs-laser excitation of 5d electrons in non-equilibrium warm dense Au. The results show that the electron thermalization time increases with excitation energy density, contrary to the well-known decrease of thermalization time with heating when only the conduction electrons are heated. This new behavior is attributed to the role of bound states in electron kinetics whereby electronic transitions due to photo-excitation and Auger decay dominate during the pump laser pulse and the subsequent thermalization requires the establishment of a Fermi-Dirac energy distribution of the 6s,p and 5d electrons via electron-electron scattering accompanied by collisional excitation and Auger decay.

Primary author(s) : NG, A. (Department of Physics & Astronomy, University of British Columbia, Canada)

Co-author(s) : Z. Chen[2], Y.Y. Tsui[2], M.Z. Mo[2], R. Fedosejevs[2], T. Ozaki[3], V. Recoules[4], and P.A. Sterne[5]

[2]Department of Electrical & Computer Engineering, University of Alberta, Canada
[3]INRS-EMT, University of Quebec, Canada
[4]CEA, DAM, DIF, France
[5]Lawrence Livermore National Laboratory, U.S.A.

X-ray absorption spectroscopy with a laser-produced betatron source

Exploring and understanding ultrafast processes at the atomic level is a scientific challenge. Femtosecond X-ray absorption spectroscopy (XAS) arises as an essential experimental probing method, as it can simultaneously reveal both electronic and atomic structures, and thus potentially unravel their nonequilibrium dynamic interplay which is at the origin of most of the ultrafast mechanisms. However, despite considerable efforts, there is still no femtosecond X-ray source suitable for routine experiments.

In a recent paper [1], we show that betatron radiation from relativistic laser−plasma interaction combines ideal features for femtosecond XAS. It has been used to investigate the nonequilibrium dynamics of a copper sample brought at extreme conditions of temperature and pressure by a femtosecond laser pulse. We measured a rise-time of the electron temperature below 100 fs. This experiment demonstrates the great potential of the table-top betatron source which makes possible the investigation of unexplored ultrafast processes in manifold fields of research. In particular, such resolution highlight a non-ballistic electron transport in warm dense copper (see figure), and will allow us to measure the effect of the electronic conduction in such regime.

Primary author(s) : LECHERBOURG, Ludovic (CEA)

Co-author(s) : Dr. DORCHIES, Fabien (CELIA, CNRS - CEA - Univ. Bordeaux, F-33400 Talence, France)

Simulating the ultrafast nonequilibrium electron dynamics in warm dense matter

In many warm dense matter experiments electrons are driven far away from equilbrium, and their thermalization dynamics are of high importance for the diagnostics of the plasma.
Theoretical approaches that are being applied include hydrodynamics, Born-Oppenheimer DFT, time-dependent DFT, or kinetic theory. However, important effects such as electronic quantum effects, correlations, dynamical screening and screening buildup are only partly captured by those approaches. Here we outline a quantum kinetic approach within nonequilibrium
Green functions theory [1,2]. This allows for an accurate treatment of dynamical properties such as the dynamical structure factor [3,6]. Moreover, the equilibration dynamics with time-dependent screening is accessible within the GW-approximation that extends the Balescu-Lenard equation to short time scales. Here we discuss the extension of recent results for lattice systems [4,5] to warm dense matter conditions. Finally, we discuss the inclusion of correlation effects via local field corrections where recnetly ab initio Quantum Monte Carlo data have become available [6].

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[2] K. Balzer and M. Bonitz, “Nonequilibrium Green’s Functions approach to inhomogeneous systems”
[3] N.H.Kwong and M. Bonitz, Phys. Rev. Lett. 84, 1768 (2000) [4] K. Balzer, M. Rodriguez
Rasmussen, N. Schlünzen, J.-P. Joost, and M. Bonitz, Phys. Rev. Lett. 121, 267602 (2018)
[5] J.-P. Joost, N. Schlünzen, and M. Bonitz, Phys. Stat. Sol. (b) article No. 1800498 (2019)
[6] T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, Phys. Rev. Lett. 121, 255001 (2018)

Primary author(s) : Dr. BONITZ, Michael (Uni Kiel)

Study of Mixtures Across the Warm-Dense-Matter Regime

We present work that looks at the behavior of multi-component mixtures and their transport properties. First, we look at a three component mixture of H-Ag and several different intermediate ion species ranging from D and Rb. This study shows us how the charge state and mass of the intermediate particle impacts the transport properties of the system. As a second topic, we look at a molecular mixtures. Here we study both the liquid and solid behavior of the systems. We use various techniques to understand these mixtures such as transport properties and bonding analysis. We also consider how to generate the molecular EOS in a flexible and reliable way as the composition varies.

Primary author(s) : TICKNOR, Christopher (Los Alamos National Laboratory)

Development of Finite-Temperature Exchange-Correlation Functionals: Improving Reliability for Warm-Dense-Matter Applications

Thermal density functional theory (DFT) is one of the standard tools in high- energy-density physics used to determine the fundamental properties of matter under extreme conditions, especially in warm dense regime when quantum effects are essential. One of the challenges of conventional implementation is that zero-temperature exchange- correlation (XC) functionals do not take into account thermal effects. This talk will address this challenge, discuss details of the formal development of new generalized-gradient approximation XC free-energy functional which bridges low-temperature (ground-state) and high-temperature (plasma) limits [1], and report main results. In particular we found that XC thermal effects account for softening of the deuterium Hugoniot at pressures P > 250 GPa and improve agreement with recent experimental measurements [2]. Calculated reflectivity of shocked deuterium along the Hugoniot is in good agreement with recent experimental measurements on the OMEGA Laser System. The dc conductivity is increased by ˜4% because of XC thermal effects. Therefore, XC thermal effects must be taken into account for accurate predictions of matter properties in the warm dense regime.

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[1] V. V. Karasiev, J. W. Dufty, and S. B. Trickey, Phys. Rev. Lett. 120, 076401 (2018).
[2] V.V. Karasiev et al., “Exchange-Correlation Thermal Effects in Shocked Deuterium:
Softening the Principal Hugoniot and Thermophysical Properties,” to be submitted to
Physical Review B.

Primary author(s) : Dr. KARASIEV, Valentin (Laboratory for Laser Energetics, University of Rochester)

Co-author(s) : Dr. HU, Suxing (Laboratory for Laser Energetics, University of Rochester)

Ab Initio Path Integral Monte Carlo Results for the Dynamic Structure Factor of Correlated Electrons:
From the Electron Liquid to Warm Dense Matter

Over the last decades, there has emerged a growing interest in warm dense matter (WDM), an exotic state with extreme densities and temperatures. These conditions are relevant for the description of astrophysical objects like brown dwarfs and giant planet interiors, meteor impacts, and laser-excited solids. In addition, WDM occurs on the pathway towards inertial confinement fusion, which promises a potential abundance of clean energy in the future.
Despite the remarkable experimental progress at large research facilities around the globe, a thorough theoretical description of WDM is notoriously difficult due to the complicated interplay of (1) Coulomb coupling, (2) thermal excitations, and (3) quantum degeneracy effects.

In this work, we focus on the uniform electron gas (UEG), one of the most fundamental model systems in physics and quantum chemistry. Although most ground state properties of the UEG have been known for decades, a full thermodynamic description at WDM conditions has only been achieved recently [1] on the basis of ab initio quantum Monte Carlo simulations [2,3]. In this contribution, we extend these considerations to the dynamic structure factor—the key quantity in X-ray Thomson scattering (XRTS) experiments, which have emerged as a standard tool of diagnostics in WDM experiments [4].
More specifically, we have carried out extensive path integral Monte Carlo simulations of the UEG going from WDM conditions to the strongly correlated electron liquid regime to compute an imaginary-time density—density correlation function. The latter is subsequently used as input for a new reconstruction procedure, which allows to obtain ab initio results for the dynamic structure factor including all exchange-correlation effects [5]. While the required inverse Laplace transform is notoriously difficult and, in fact, ill-posed, this problem is rendered tractable by a novel stochastic sampling scheme of the dynamic local field correction, which allows to fulfill a number of exact properties.
This has allowed us to compute the first accurate data for the dynamic structure factor for different densities and temperatures, and to gauge the accuracy of previous approximations. Interestingly, at strong coupling we find nontrivial shapes around intermediate wave vectors, which manifest in a negative dispersion relation. We expect our results to be of direct interest for, e.g., the interpretation of XRTS experiments and as input for other methods like quantum hydrodynamics and time-dependent density functional theory.

[1] S. Groth, T. Dornheim, T. Sjostrom, F. Malone, WMC Foulkes, and M. Bonitz, Phys. Rev. Lett. **119**, 135001 (2017)
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[3] T. Dornheim, S. Groth, T. Sjostrom, F. Malone, WMC Foulkes, and M. Bonitz, Phys. Rev. Lett. **117**, 156403 (2016)
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[5] T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, Phys. Rev. Lett. **121**, 255001 (2018)

Primary author(s) : Dr. DORNHEIM, Tobias (Kiel University)

Co-author(s) : Dr. GROTH, Simon (Kiel University); Dr. VORBERGER, Jan (HZDR); Prof. BONITZ, Michael (Kiel University)

Thermodynamics of Shock and Isentropic Compression of Warm Dense Matter

The behavior of matter at extremely high pressures is very interesting for understanding the structure and evolution of astrophysical objects and many modern energy technologies.
Dynamic methods of generation of warm dense matter at extremely high pressures, based on the compression and heating of matter in intensive shock waves, adiabatic expansion of preliminary compressed samples and quasiisentropic compression are discussed. To generate shock waves in the terapascal pressure range, the cylindrical and spherical high explosives, laser and heavy low beams, high velocity impacts, and soft X-rays were used. The fast diagnostics of the extreme states of warm dense matter were elaborated - differential laser indicators of velocity, fast electron-optical cameras, pyrometers, and high-speed spectrometers equipped with the optical fibers transmission lines. The experimental data were obtained and the physical models of warm dense matter behavior at extremely high pressures, temperatures and deformation rates were proposed. These are - the metallization and dielectrization of strongly compressed hot matter, high energy density thermodynamics and warm matter transitions. Shear viscosity of matter as an indicator of particles correlations in a wide region of parameters from Plank’s scale to laboratory conditions is analyzed.

Primary author(s) : Prof. FORTOV, Vladimir E. (Joint Institute for High Temperatures of RAS)

The High-Pressure Melting Line and Band-Gap Closure in Helium

We study the behavior of solid and liquid helium at high pressure with molecular dynamics simulations based on density functional theory (DFT-MD). Helium, the second abundant element, is important in astrophysics, e.g., for the interior and evolution of gas giants and brown dwarfs. In particular, we calculate the melting line and examine the insulator-to-metal transition up to TPa pressures. For the calculation of the melting line we use two-phase simulations [1]. We find good consistency with experiments and give predictions for the helium melting line up to the TPa region.
Laser-driven compression experiments have shown that helium undergoes an insulator-tometal transition with increasing density and temperature [2]. However, the exact location and nature of this transition is not clear yet. Recent theoretical predictions for the band-gap closure in helium [3, 4] differ within a factor of two in density. Based on extensive DFT-MD simulations we find good agreement with the results of Zhang et al. [4].

[1] Robert et al., “Simple calculation of ab initio melting curves: Application to aluminum”,
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[4] W. Zhang et al., “Revisiting metallization boundary of warm dense helium in a wide r-T
regime from ab initio study”, Sci. Rep. 7, 41885 (2017).

Primary author(s) : PREISING, Martin (University of Rostock)
Co-author(s) : Prof. REDMER, Ronald (Universität Rostock)

Polymorphism, amorphization and melting of shocked MgSiO3 from in situ X-ray diffraction

Constraining shock-induced transformations of major silicates and their kinetics is necessary to constrain planetary formation models of the terrestrial planets and to understand how meteorites have been affected by repetitive shocks. The recent coupling of ultrafast in situ X-ray diffraction (XRD) and shock compression techniques (gas guns and laser facilities) enables the direct investigation of transition mechanisms at short time-scales (from hundreds of picoseconds to hundreds of nanoseconds). In this study, we probed the structure at peak pressure of shocked MgSiO3 glass and orthoenstatite single crystals up to 1-3 Mbar by coupling ultrafast XRD to laser-driven shock compression at LCLS MEC end-station of SLAC XFEL facility (Stanford, USA). Shocked MgSiO3 glass presents typical features of six-fold Si-O coordinated amorphous silicate. At a given pressure its structure is similar to what has been observed in high-pressure glass at 300 K in static compression experiments. We report no evidence of bridgmanite (Bd) or MgSiO3 post-perovskite (Ppv) at nanosecond time-scale.

Instead we found that shocked enstatite amorphizes below the equilibrium melting. This observation indicates a slower kinetic of transformation in shocked MgSiO3 than in shocked SiO2 glass, which may result from a high configuration entropy in amorphous MgSiO3 and from the slow diffusion of Mg cations. The structure of the metastable amorphous phase is compared to the melt obtained at higher pressures and also presents typical features of highly coordinated silicate. Comparing temperature estimations of the amorphous state obtained in this study and existing gas-gun measurements, we provide indirect evidence that crystallization of MgSiO3 Ppv may occur at microsecond-scale in shocked enstatite above 150 GPa and below the equilibrium melting.

Primary author(s) : Dr. HERNANDEZ, Jean-Alexis (Laboratoire d’Utilisation des Lasers Intenses, Ecole Polytechnique)

Co-author(s) : Dr. MORARD, Guillaume (Sorbonne Université, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, Museum National d’Histoire Naturelle, UMR CNRS); Mr. GUARGUAGLINI, Marco (Laboratoire LULI, Ecole Polytechnique); Dr. ALONSO-MORI, Roberto (SLAC National Accelerator Laboratory) Dr. BENUZZI-MOUNAIX, Alessandra (Laboratoire pour l’Utilisation des Lasers Intenses (LULI), Ecole Polytechnique, CNRS, CEA, UPMC); Dr. BOLIS, Riccardo (Laboratoire pour l’Utilisation des Lasers Intenses (LULI), Ecole Polytechnique, CNRS, CEA, UPMC); Dr. FIQUET, Guillaume (Sorbonne Université, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, Museum National d’Histoire Naturelle, UMR CNRS); Dr. GALTIER, E. (SLAC National Accelerator Laboratory); Dr. GLEASON, Arianna (Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory); Dr. GLENZER, S. (SLAC National Accelerator Laboratory); Dr. GUYOT, François (Sorbonne Université, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, Museum National d’Histoire Naturelle); Dr. KO, B. K. (School of Earth and Space Exploration, Arizona State University); Dr. LEE, H. J. (SLAC National Accelerator Laboratory); Dr. MAO, W. L. (Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory); Dr. NAGLER, B. (SLAC National Accelerator Laboratory); Dr. OZAKI, N. (Graduate School of Engineering, Osaka University and Institute of Laser Engineering, Osaka University); Ms. SCHUSTER, Anja (Helmholtz-Zentrum Dresden-Rossendorf, Germany); Dr. SHIM, S. H. (School of Earth and Space Exploration, Arizona State University); Dr. VINCI, Tommaso (Laboratoire pour l’Utilisation des Lasers Intenses (LULI), Ecole Polytechnique, CNRS, CEA, UPMC); Dr. RAVASIO, Alessandra (Laboratoire pour l’Utilisation des Lasers Intenses (LULI), Ecole Polytechnique, CNRS, CEA, UPMC,)

Properties of water under ultrahigh pressure by combining DAC static and high power laser dynamic loading

Water is thought to be one of the most abundant compounds of the mantles of “icy” giant planets like Uranus and Neptune. The temperature and the pressure of the Neptune mantle are estimated to about 5000 K and 300 GPa, respectively. Therefore, properties (equation of state, temperature, reflectivity, conductivity, etc.) of water relevant to “icy” giant planets’ mantle conditions are of great importance for studying the formation, evolution, structure, composition, and the magnetic field of these planets. We combine diamond anvil cell (DAC) static and high power laser dynamic techniques for compressing water to the Neptune mantle condition, and study water properties. According to the loading characteristics of SG-[U+2161]high power laser facility, a new DAC adapted for high power laser dynamic loading is developed. Water can be compressed by DAC firstly (static pressure is up to 1.2 GPa), then be compressed by laser-driven shocks (dynamic pressure is up to 400 GPa). The equation of state, temperature, sound velocity, reflectivity, and the conductivity of water under above pressure conditions were obtained. Our data totally agree with those of the model based on quantum molecular dynamics (QMD) calculations.

Primary author(s) : Prof. HUANG, Xiuguang (Shanghai Institute of Laser Plasma)

Sound velocity of quasi-isentropic compressed dense deuterium up to Mbar pressure

Two-stage light-gas gun-driven multiple shock reverberation compression experiments were designed and performed to probe thermodynamics properties of deuterium ranging from the initial 40 MPa up to Mbar pressure. The time-resolved optical radiation histories and interface velocity profiles were simultaneously measured in a single shot by a joint diagnostics of multichannel optical pyrometer (MCOP) and Doppler Pin System (DPS). These measurements were used to diagnose the thermodynamics states of the multi-compressed deuterium. The up to 10 times shock, for deuterium, was successfully observed, which covered a wide pressure range of 1-120 GPa. It was found that the deuterium, starting from the fourth-shock, undergoes a quasi-isentropic compression path. Thus, the quasi-isentropic sound velocity of the dynamically compressed deuterium can be deduced via Cs=[(@P/@r)s]ˆ(0.5) based on the experimentally obtained P-r data. The results were analyzed by using a self-consistent fluid variational theory (SFVT) model. The sound velocity data on deuterium under quasiisentropic compression have potential applications in constructing accurate models for the interiors structure of the gaseous giant planets and enriching the understanding on properties of warm dense matter.

Primary author(s) : Dr. YUNJUN, Gu (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China)

Co-author(s) : Prof. QIFENG, Chen (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China); Dr. GUOJUN, Li (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China); Dr. CHENGJUN, Li (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China); Dr. YUFENG, Wang (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China); Dr. ZHIGUO, Li (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China); Dr. LEI, Liu (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China); Dr. YI, Mu (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China); Dr. ZHAOQI, Wang (National Key Laboratory of Shock Wave and Detonation Physics, Institute of Fluid Physics, China)

Ab initio study of Iron-Nickel alloys in Super-Earths cores

Iron-nickel alloys are considered the main components of Earth and Super-Earth cores, which make them crucial systems in order to comprehend the properties of these planets. While the relative nickel content is anticipated to be around 10% in the Earth, this value could differ slightly in other planets because of different host star metallicity and formation history. It is thus important to understand the properties of iron-nickel systems with various compositions in the multi-megabar regime. While pure iron is anticipated to have hexagonal close packing at high pressure, nickel is expected to have face-centered cubic packing. This means there is a structural change as the composition is modified, which can also mean a limited stability of the solid solutions of iron-nickel. We will discuss the properties of iron-nickel alloys in the megabar regime as predicted by *ab initio* simulations. We will examine the relative stability of different iron-nickel solid solution compositions and the interplay of the spin states. After characterizing the properties of these alloys at pressure-temperature conditions relevant for Super-Earth, we will discuss possible consequences their cores.

Primary author(s) : Dr. SOUBIRAN, François (ENS Lyon)
Co-author(s) : Dr. CARACAS, Razvan (LGLTPE ENS Lyon)

Non-equilibrium electron kinetics in warm dense Au

Electron kinetics plays a central role in the transformation of a cold solid to warm dense matter via ultrasfast heating as it governs the evolution of the electronic structure of the state. A notable case is the heating of Au with fs-laser radiation that has been a longstanding platform for WDM studies. Specifically, single-photon absorption of 400nm laser light leads to photo-excitation of the 5d electrons. The excitation rate is dictated by the rate of energy deposition by the pump laser pulse. This is accompanied by rapid Auger decay of the resulting 5d holes, thus creating a strongly-out-of-equilibrium electron system. Its relaxation towards an equilibrium occupation of the valence bands then occurs via the balance between collisional excitation and Auger decay while a Fermi-Dirac electron energy distribution will be established in electron-electron scattering. The behavior of non-equilibrium electron kinetics can be observed from the temporal evolution of ac conductivity. This was demonstrated in an earlier experiment using a 400nm, 48fs (FWHM) pump laser pulse and an 800nm, 51fs (FWHM) probe laser pulse. For an excitation energy density of 4.3MJ/kg (0.83x1011J/m3), observations yielded (i) a lifetime of ˜10fs for the 5d holes produced by photo-excitation and (ii) an electron thermalization time of ˜300fs. Here, we report on a new study in which the duration of photo-excitation is reduced to 10fs with a commensurate 5-fold increase in photo-excitation rate. Equally significant, the temporal resolution of the measurements is enhanced by more than 5-fold to 8fs. In addition to the new experimental findings, electron kinetics calculations based on a rate-equation method will also be discussed.

Primary author(s) : WANG, X. (1Department of Physics, National University of Defense Technology, China)
Co-author(s) : C. Gao[1], D.Zhang[1], R. Zhang[2], S. Zhang[1], Y. Hou[1], J. Dai[1], Z. Zhao[1], J. Yuan[1], Y.Y. Tsui[2] and A. Ng[3]
[1]Department of Physics, National University of Defense Technology, China
[2]Department of Electrical, Computer Engineering, University of Alberta, Canada
[3]Department of Physics & Astronomy, University of British Columbia, Canada

Ab initio calculation of electron impact ionization for ions in exotic electronic configurations

X-ray free-electron lasers (XFELs) provide intense femtosecond pulses of hard x rays, which are used, in particular, for studies of laser-created plasmas and ultrafast coherent diffraction imaging. Upon interaction with the sample under consideration, the x rays photoionize electrons, and, in particular, also inner-shell electrons [1]. The resulting core-hole states undergo ultrafast decay via various channels, including fluorescence and Auger decay, the latter of which is the predominant relaxation channel for light elements, and typically takes place on a scale of 1-10 fs [1]. At this timescale, however, the core-hole ions may undergo electron-impact ionization, due to the abundance of highly energetic photoelectrons, and Auger electrons. In this study, we provide an ab initio calculation of the electron-impactionization cross sections of ions at zero temperature [2]. This allows us to compare the impact- ionization cross sections of ions in exotic electronic states (with core holes), which may be formed during the interaction with intense XFEL pulses, and ions in their respective ground states. The ab initio framework which we employed allows for these calculations to be easily incorporated in other types of simulation codes, including non-equilibrium formation of x-ray-created plasmas.

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cross sections for ions in exotic electron configurations,” Phys. Rev. A 98, 022701
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Primary author(s) : BEKX, John Jasper (CFEL/DESY)

Co-author(s) : Dr. ZIAJA-MOTYKA, Beata (HASYLAB); Dr. SON, Sang-kil (CFEL-DESY); Prof. SANTRA, Robin (CFEL-DESY)

Dynamics and Properties of High-Density Surface Plasmas Induced by Cold X-rays

The interaction of intense energy fluxes such as particle or laser beams with the surface of materials results in the formation and ultrafast spatiotemporal evolution of Warm Dense Plasmas (WDPs). The prediction of rapidly evolving and highly non-equilibrium WDPs is very challenging for computational models. The steep spatial gradients, rapid temporal variations of the WDP state, and uncertainty of energy sources due to the lack of a dominating energy scale should be considered. Our research is focused on predicting and understanding the formation, spatiotemporal evolution, physical and electrical properties of highly transient WDPs produced by cold X-rays on the surface of solar panels of satellites from high altitude nuclear detonations. Implications of X-ray irradiation of solar cells are potentially quite serious. The density of WDP near the surface can approach the density of a solid. Electron temperature in WDP is in the range of 1-5 eV. The damage can be caused by this expanding dense plasma in the gap between adjacent cells by short-circuiting the cells.
A computational model coupling the Monte Carlo (MC) and Molecular Dynamics (MD) methods with the Hartree-Fock-Slater - Collisional-Radiative Steady-State (HFS-CRSS) model is developed. The unique capabilities of a combination of discrete and continuum computational approaches are applyed to predict X-ray absorption by materials, WDP formation and expansion, composition and optical properties of warm high-density plasmas. The spatial distribution of energy deposited by cold X-rays with blackbody spectrum into materials of solar cells is evaluated using the MC model. The energy deposition profiles are then used in the atomistic MD model to predict the spatiotemporal evolution of WDP in vacuum. The time-dependent information on the spatial distribution of density, temperature, and pressure fields of expanding WDP is derived from the MD simulations. The plasma density and temperature distributions are used in the HFS-CRSS model as input data for predicting the composition of ion species, concentration of free electrons, absorption and emission coefficients of WDP. These modeling results provide insights into the underlining physics of the formation and spatiotemporal evolution of WDPs induced by cold X-rays.

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Primary author(s) : Prof. MILOSHEVSKY, Gennady (Virginia Commonwealth University)
Co-author(s) : FOGLEMAN, Myles (Virginia Commonwealth University); WENZEL, Cole (Virginia Commonwealth University)

Surface dynamics of solids upon high-intensity laser irradiation investigated by grazing incidence X-ray surface scattering

The ability to visualize surface dynamics upon short-pulse high-intensity laser irradiation in femto-second and nano-meter scale is not only of fundamental scientific interest, in fields as diverse as material processing, warm dense matter and relativistic laser-plasma interaction, but also provides the basis for technological developments that benefit from transient shape of surface plasmas; ranging from simple plasma reflective opics to high-orderharmonic generation for atto-second XUV pulse generation. Currently available optical probe techniques are often limited by its spatial resolution and its insensitivity to solid density. We have performed first proof-of-principle experiment using grazing incidence X-ray surface diffuse scattering at the SACLA X-ray free electron laser facility in Japan. We studied dynamically changing solid surface structure upon medium-intensity (10^14 – 10^16 W.cm^-2) laser irradiation with a few nanometer in-plane and in-depth resolution simultaneously. By varying the laser-pump and X-ray probe delay, we successfully measured the dynamics of initial compression and subsequent evaporation of surface layers upon laser irradiation in single shot, thanks to high-intensity short-pulse X-ray beam. The results will yield unique insights into the surface dynamics as well as provide invaluable benchmarking for simulations at highly non-equilibrium, warm dense plasmas. In this talk, we report our experimental observation, various simulation results, and applicability of this new technique for future applications.

Primary author(s) : Dr. NAKATSUTSUMI, Motoaki (European XFEL)
Co-author(s) : Mr. BANJAFAR, Mohammadreza (European XFEL GmbH); Ms. RANDOLPH, Lisa (University of Siegen); Dr. YABUUCHI, Toshinori (RIKEN, SPring-8 Center, Japan); Dr. DOVER, Nicholas (Kansai Photon Science Institute, QST, Kyoto); Dr. GÖDE, Sebastian (European XFEL); Dr. INUBUSHI, Yuichi (JASRI, Hyogo, Japan); Dr. JAKOB, Gerhard (Universität Mainz); Mr. KAA, Johannes (European XFEL); Prof. KLÄUI, Mathias (Universität Mainz); Dr. KON, Akira (QST, Kyoto, Japan); Dr. KOGA, James (QST, Kyoto, Japan); Dr. KSENZOV, Dmitriy (Universität Siegen); Dr. MAKITA, Mikako (European XFEL); Dr. MATSUOKA, Takeshi (Osaka University, Japan); Dr. NISHIUCHI, Mamiko (QST, Kyoto, Japan); Dr. PRESTON, Thomas (European XFEL); Dr. RÖDEL, Christian (Jena); Mr. SCHON, Frederic (Universität Siegen); Dr. SUEDA, Keiichi (JASRI, Hyogo, Japan); Prof. SENTOKU, Yasuhiko (Osaka University, Japan); Dr. TADASHI, Togashi (JASRI, Hyogo, Japan); Dr. VAFAEE-KHANJANI, Mehran (Universität Mainz); Dr. BUSSMANN, Michael (Helmholtz-Zentrum Dresden - Rossendorf); Prof. COWAN, Thomas (HZDR, Germany); Dr. FORTMANN-GROTE, Carsten (European XFEL); Dr. KLUGE, Thomas (HZDR); Dr. MANCUSO, Adrian (European XFEL); Dr. ZASTRAU, Ulf (European XFEL /HED); Prof. CHRISTIAN, Gutt (Universität Siegen)

Measuring Plasma Parameters of Warm Dense Matter from X-Ray Thomson Scattering at the LCLS and the NIF

The thermal and electrical conductivity, equation of state and the spectral opacity in warm dense matter (WDM) are essential properties for modeling, e.g., fusion experiments or the evolution, interior and magnetic field generation of planets. In the last decade, it has been shown that x-ray Thomson scattering (XRTS) is an effective tool to determine plasma parameters like temperature and density in the WDM regime [1]. Recently, the electrical conductivity was extracted from XRTS experiments for the first time [2]. The spectrally resolved scattering data of aluminum, isochorically heated by the Linac Coherent Light Source (LCLS), show strong dependence on electron correlations. Therefore, the damping of plasmons, the collective electron oscillations, has to be treated beyond perturbation theory. Furthermore, an ongoing experimental campain at the National Ignition Facility (NIF) measures XRTS spectra of imploding beryllium capusules for the first time in forward direction under extreme conditions, i.e. beyond 20 times compression.

We present results for the dynamic transport properties in warm dense aluminum and beryllium using density-functional-theory molecular dynamics (DFT-MD) simulations. The choice of the exchange-correlation (XC) functional, describing the interactions in the electronic subsystem, has significant impact on the ionization energy of bound electrons and the dynamic dielectric function. Our newly developed method for the calculation of XRTS signals including plasmon and bound-free transitions is based on transition matrix elements together with ionic contributions using uniquely DFT-MD simulations. The results show excellent agreement with the LCLS data if hybrid functionals are applied [3]. The experimental finding of nonlinear plasmon damping is caused by the non-Drude conductivity in warm dense aluminum. Here, we show further validation by comparing with x-ray absorption data [4]. These findings enable new insights into the impact of XC functionals on calculated properties of WDM and allow detailed predictions for ongoing experiments at the extreme densities reached at the NIF.

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Primary author(s) : Prof. REDMER, Ronald (Universität Rostock)
Co-author(s) : Mr. WITTE, Bastian, Bernhard, Lothar (Rostock University, SLAC); Dr. BETHKENHAGEN, Mandy (Universität Rostock); Dr. RECOULES, Vanina (CEA, DAM, DIF, France); Dr. SPERLING, Philipp (aible GmbH Rostock); Dr. FRENCH, Martin (Universität Rostock); Dr. DOEPPNER, Tilo (Lawrence Livermore National Laboratory); Prof. GLENZER, Siegfried H. (SLAC National Accelerator Laboratory, USA)

Characterising the icy giant planets’ interiors via laser-driven shock compression of water, ammonia, and a C:H:N:O mixture

Water, ethanol, and ammonia are amongst the key components of Uranus and Neptune.

Knowing their equation of state, conductivity, and transport properties at planetary interiors conditions (pressures of several megabar, temperatures of a few thousand Kelvin) is required for developing precise models of the two planets, with the aim of explaining their puzzling structures, magnetic fields, and luminosities. The physical and chemical behaviour of such mixtures at extreme pressures and temperatures is not only important for planetology but also interesting on its own, since those conditions are characterised by the coexistence of dissociated atoms, atomic clusters and chains. This regime is very difficult to study via ab initio simulations and experimental verifications are thus required.
Using laser-driven shocks, we compressed up to 3 Mbar pure water, pure liquid ammonia, and a C:H:N:O mixture composed by water, ethanol, and ammonia. Their principal Hugoniot curves have been explored using the decaying shock technique. Moreover, off-Hugoniot states have been reached via a double-shock technique and through the coupling of dynamic andstatic compression in diamond anvil cells. The experiments were performed at the LULI2000 laser facility using standard rear-side optical diagnostics (VISARs, SOP). The equation of state and the optical reflectivity of the shock front have been measured, allowing an estimation of the electrical conductivity.
The results show that water and C:H:N:O mixtures share the same equation of state with a trivial density scaling, while the reflectivity behaves differently in both the onset pressure and the saturation value. The experimental study of the structural and optical properties of shock-compressed ammonia confirms the predictions of recent ab initio simulations. The consequences for the modelling of the interiors of the icy giant planets will be discussed.

Primary author(s) : GUARGUAGLINI, Marco (Laboratoire LULI, École Polytechnique)
Co-author(s) : Dr. HERNANDEZ, Jean-alexis (Laboratoire LULI, École Polytechnique); Mr. LEFEVRE, Frédéric (Laboratoire LULI, École Polytechnique); Dr. NINET, Sandra (IMPMC - Sorbonne Université); Dr. DATCHI, Frédéric (IMPMC - Sorbonne Université); Dr. VINCI, Tommaso (Laboratoire LULI, École Polytechnique); Dr. BENUZZI-MOUNAIX, Alessandra (Laboratoire LULI, École Polytechnique); Dr. RAVASIO, Alessandra (Laboratoire LULI, École Polytechnique)

Thermodynamic properties of C-N-O-H mixture in the region of non-ideal plasma

The atmosphere of giant planets in the Solar System, such as Uranus and Neptune, consists of mixed water, ammonia, and methane heated to the state of warm dense matter. All these compounds have rather complicated phase diagrams which include some exotic structures, e.g. super-ionic water. A physically consistent description of all interactions in such mixtures can only be attained from first principles. The non-empirical methods, such as quantum molecular dynamics (QMD), are however strongly limited both in the dimensions of systems which can be modeled, and in the times during which their evolution can be tracked. We try to tackle these problems by modifying the classical reaction potential ReaxFF [1] on the basis of the pair correlations functions obtained in QMD calculations. Here we investigate how the calculated thermodynamic properties of mixed carbon, nitrogen, oxygen and hydrogen depend on ReaxFF parameters for systems of several tens of thousand atoms, and do comparisons with similar results obtained from first principles for much smaller systems.

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Primary author(s) : Dr. RYKOUNOV, Alexey (Russian Federal Nuclear Center – Academician E.I. Zababakhin All-Russian Research Institute of Technical Physics (RFNC-VNIITF))
Co-author(s) : Mrs. VOROBYOVA, Marina (Russian Federal Nuclear Center - All-Russian Institute of Technical Physics)

Multiple shock reverberation compression of dense Ne up to warm dense regime: evaluating the theoretical models

Multiple shock reverberation compression experiments are designed and performed to determine the equation of state of neon ranging from the initial dense gas up to the warm dense regime, where the pressure is from about 40 MPa to 120 GPa and the temperature is from about 297 K up to above 20000 K. The wide region experimental data are used to evaluate the available theoretical models. It is found that, for neon below 1.1 g/cm3, within the framework of density functional theory molecular dynamics, a van der Waals correction is meaningful. Under high pressure and temperature, results from the self-consistent fluid variational theory model are sensitive to the potential parameter and could give successful predictions in the whole experimental regime if a set of proper parameter is employed.
The new observations on neon under megabar pressure and eV temperature enrich the understanding on properties of warm dense matter, and have potential applications in revealing the formation and evolution of gaseous giants or mega-Earths.

Primary author(s) : Dr. TANG, Jun (Science and Technology on Surface Physics and Chemistry Laboratory)

Observation of Nonlocal Electron Transport in Warm Dense CH

We present the first observation of nonlocal electron transport in Warm Dense Matter (WDM) in an experiment carried out at the OMEGA laser facility. Low-density CH foam was compressed by a 2 ns laser drive at _ 7×10^{14} W/cm^2 generating WDM conditions in a compression wave. Increased plasma heating within (17 – 35 eV) and ahead of the compression wave and significantly faster shock with a rapidly decaying velocity profile were observed by a combination of independent diagnostics including X-ray Thomson Scattering (XRTS), velocity interferometry (VISAR) and streaked optical pyrometry (SOP). Comparison with radiation hydrodynamics simulations using the PETE code with an explicit treatment of nonlocal electron transport confirm that these experimental observations are consistent with nonlocal electron transport as the Knudsen number exceeds the threshold of 0.001 in the preheat region close to the compression wave.

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Primary author(s) : Dr. FALK, Katerina (Helmholtz-Zentrum Dresden-Rossendorf)
Co-author(s) : Dr. HOLEC, Milan (Lawrence Livermore National Laboratory); Dr. FONTES, Christopher J. (Los Alamos National Laboratory); Dr. FRYER, Christopher L. (Los Alamos National Laboratory); Dr. GREEFF, Carl W. (Los Alamos National Laboratory); Dr. JOHNS, Heather M. (Los Alamos National Laboratory); Dr. MONTGOMERY, David S. (Los Alamos National Laboratory); Mr. SCHMIDT, Derek W. (Los Alamos National Laboratory); Dr. ŠMÍD, Michal (Helmholtz-Zentrum Dresden-Rossendorf)

Using intense laser-driven proton beams to produce warm, dense materials

Chirped pulse amplified lasers have reached the kilojoule-petawatt class, and the secondary sources of radiation they produce are themselves now capable of driving unexplored physics.
Laser-driven proton beams with MeV to 10s of MeV particle energy and 10s of J beam energy can now be the pump in innovative experiments such as isochoric heating to warm (>100 eV), dense matter states. The beams are orders of magnitude more intense than bunches at conventional accelerator facilities due to their picoseconds duration and waist <100 microns, leading to complex interactions when entering solid materials. This talk will describe experimental methods for delivering intense proton beams to heat a secondary target to warm and hot dense matter conditions and describe attempts to better characterize the resulting matter through x-ray spectroscopic techniques. I will also showcase simulations by my colleagues that investigate intensity-dependent transport phenomena using warm dense matter stopping power models in targets including unexpanded solids and near-solid density foams.

Primary author(s) : Chris McGuffey (University of California San Diego)

Electronic Transport Properties of Warm Dense Matter from Time-dependent Density Functional Theory

Understanding the high energy density plasmas generated on pulsed power facilities (Z machine) and at coherent light sources (European XFEL, LCLS) requires interpreting complex diagnostic signals such as fluorescence emission and x-ray scattering emission. Predicting their evolution requires adequate models of transport properties in extreme (and extremely non-equilibrium) states of matter. Here, we present time-dependent density functional theory (TDDFT) calculations of electronic transport properties (dielectric function, electrical conductivity, and absorption c oefficient) in aluminum and copper under ambient, isochorically heated and shock-compressed conditions. We compare the utility of TDDFT with other state-of-the-art approaches such as the Kubo-Greenwood formalism and average-atom models in terms of accuracy, computational cost, and self-consistency.

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Primary author(s) : Dr. CANGI, Attila (Sandia National Laboratories)
Co-author(s) : Dr. BACZEWSKI, Andrew (Sandia National Laboratories); HANSEN, Stephanie (SNL)

A theoretical simulation for nonequilibriumelectronic kinetics of warm dense gold

A theoretical model is developed to simulate the ultrafast non equilibrium electronic kinetics of goldin warm dense regime, which is heated by a 400 nm laser pulse with 10 fs duration. The populations of atomic levels are obtained by solving a time-dependent rate equation, which includes the main microscopic atomic processes such as photoexcitation, Auger decay and electron impact ionization. The atomic rates are carefully determined by including the effects of atomic level broadening insuch dense matters. The electron energy distribution function (EEDF) around the Fermi level is determined by solving an isotropic Fokker-Planck equation and the ultrafast evolution of EEDF is investigated. The absorption coefficient at the wavelength of 800 nm is calculated.

Primary author(s) : Dr. GAO, Cheng (National University of Defense Technology)
Co-author(s) : Dr. DAI, Jiayu (National University of Defense Technology);Dr. HOU, Yong(National University of Defense Technology);Dr. ZENG, Jiaolong (National University of DefenseTechnology);Prof. ZHAO, Zengxiu (national university of defense technology);Prof. YUAN, Jianmin(Graduate School, China Academy of Engineering Physics);Prof. NG, Andrew (University of BritishColumbia

Electron-ion coupled dynamics of warm dense matter

Dynamics of quantum electrons and coupled ions are theoretically pivotal and challenging for the non-equilibrium processes in warm dense matter. In this talk, we firstly show the electron-ion relaxation in warm dense hydrogen using Constrained electron force field (CEFF) molecular dynamics [1]. In CEFF, quantum collisions are included since the electrons are treated as Gaussian wave packets, and the Coulomb Catastrophe in classical MD can be avoided. The results of CEFF show that the temperature relaxation time can be up to 3 times longer than that from current popular models and classical MD. The analyses of particle distributions, kinetic and potential energies, mean free path show that quantum degeneracy, delocalization, and cross sections of electrons with coupled ions are the intrinsic physics for the extremely low energy exchange rates in large-angle collisions and quantum electrons dominated warm dense matter. Furthermore, we will show the effect of electron-ion collisions on the dynamical structure factor (DSF) of warm dense matter. We will see the increase of Rayleigh peak in DSF with increasing the electron-ion collisions.[2]

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Primary author(s) : Dr. DAI, Jiayu (National University of Defense Technology)
Co-author(s) : Dr. MA, Qian (National University of Defense Technology); Dr. ZHAO, Zengxiu (National University of Defense Technology); Mr. GAO, Tianyu (National University of Defense Technology); Dr. CHOI, Yongjun (Michigan State University); Dr. MURILLO, M. S.(Michigan State University)

Time-resolved Electrical Conductivity of Warm Dense Gold Measured by Multi-cycle THz Radiation

Electrical conductivity, as a manifestation of both of both electronic and structural properties of materials, is central to the understanding of warm dense matter [1]. With the advent of ultrafast lasers, electrical conductivity at optical frequency of warm dense matter was resolved temporally at isochoric conditions well before hydrodynamic expansion occurred [2-3]. Although efforts were made to extrapolate DC electrical conductivity from optical conductivity [1], direct measurement of such intrinsic transport property with ultrafast resolution is still missing.

Recently, we employed the high brightness, multi-cycle THz radiation generated from the accelerator at FLASH to study the electrical conductivity of warm dense gold excited by XUV pulses. Owning to its much lower oscillation frequency than that of electron scattering in warm dense gold, THz radiation offers a direct approach to DC conductivity. Incorporating with the single-shot electro-optics sampling technique [4-5], continual evolution of electrical conductivity is determined with sub-picosecond resolution in a single shot. Compared with previous measured optical conductivity [3], an ultra-broadband Drude-like behavior is found in warm dense gold. The time-resolved measurement also enables us to estimate the electron scatter frequency as a function of electron and ion temperatures individually.

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Primary author(s) : Dr. CHEN, Zhijiang (SLAC National Accelerator Laboratory)

Dynamic Band Occupation and Optical Response of Warm Dense Gold

The excitation of metals with short-pulse lasers is an often applied method to create warm dense matter states. Here, the energy input drives the electronic system far out of equilibrium. The subsequent cascade of relaxation processes reveal many micro-physical properties of the system. Italso strongly influences the outcome of almost any measurement within the relaxation time. In particular, the optical response depends strongly on the occupation of electronic states within the bands, the number of electrons per band as well as the energy transfer to the ionic lattice/ion fluid. In this contribution, we investigate the behavior of gold after excitation with very short pulses of visible and VUV light that promote additional electrons from the lower bands into the conduction and. At least within the first few 100 femtoseconds, we can assume a stable lattice and thus keep the known band structure in our calculations. Firstly, we demonstrate that the number of electrons per band is sufficient to describe probing in the optical limit (k->0). Then we present a system of rate equations that describes this band occupation. For excitations with optical lasers, only d-electrons can be promoted into the sp-band and a two-band model is sufficient. With VUV light like from the FLASH laser at DESY, f-electrons can also be excited and we need a three-band model to describe the band occupation. We show similarities and differences of the two excitation methods. Based on these predictions for the band occupation, we are able to calculate the optical properties, like the reflectivity, and make predictions of the expected behavior of warm dense gold for time-resolved optical measurements.

Primary author(s) :NDIONE, P.d. (-)
Co-author(s) :S. Weber, B. Rethfeld; D.O. Gericke

Effect of an harmonicity on the hcp to bcc transition in beryllium at high pressure and high temperature conditions

We investigate the hcp to bcc phase transition in beryllium (Be) at high pressure-temperature (PT) conditions. A recently developed hybrid approach that combines first principles molecular dynamics and lattice dynamics is used to account for anharmonic contributions to the free energy. Anharmonic effects are shown to be strong at high T in both hcp and bcc Be. They are stronger in hcp Be than in bcc Be, as evidenced by the larger anharmonic vibrational entropy of hcp Be. We find that anharmonicity has a significant influence on the hcp to bcc transition at high PT conditions. It substantially enlarges the stability domain of hcp Be at high T compared with that calculated under the quasi-harmonic approximation (QHA), as a result bringing theoretical predictions into good consistency with recent experimental observations. After considering anharmonic effects, the calculated pressure and temperature of the hcp/bcc/liquid triple point increase from about 85 to 165 GPa, and from about 3300 to 4200 K, respectively, and the predicted Clapeyron slope at the triple point takes a value of −7.4 ± 0.7 K/GPa, noticeably larger in magnitude than previous QHA results in the range of -3 to 2 K/GPa.

Primary author(s) : Prof. SONG, Haifeng (IAPCM)
Co-author(s) : Dr. XIAN, Jiawei (IAPCM); Prof. YAN, Jun (IAPCM); Prof.

Kinetics and structural changes in shock-compressed bismuth

The group V metal bismuth (Bi) is well-known for exhibiting a large number of polymorphic transitions within a low pressure and temperature region [1]. the ideal candidate for such studies. Within 3 GPa it undergoes the I-II and the II-III transition and the III-V transition above 7 GPa. At high temperature, between 2.5 and 6 GPa, phase III transforms into Bi-IV. This view of the Bi-phase diagram can be drastically altered by metastable effects in static compression experiments [2], with the appearance of phase V at pressures as low as 5 GPa for example. Moreover, it was recently shown in a static study that hydrostaticity conditions have an important effect on the melting line of bismuth, which in turn is found to be much higher (the I-II-liquid triple point is found around 2.2 GPa and 490 K instead of 1.65 GPa and 465 K) [3].

Synchrotron ns time-resolved X-ray diffraction has been performed on shocked bismuth along various compression and release paths, hence exploring the Bi phase diagram up to 8 GPa and 600 K. Marked departures from the equilibrium behavior are observed. The sequence of structural changes is different upon compression and release. Bi-III, the complex host-guest structure, is never observed. Instead Bi-V is observed over a large domain. Melting of Bi-V and crystallization of the fluid into Bi-I are clearly identified on stress release.

These observations on a prototypical system underline the possible difficulties of disclosing equilibrium structural transformations at high pressure by using dynamic compression.

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Primary author(s) : Dr. PÉPIN, Charles (CEA)
Co-author(s) : Dr. MARIZY, Adrien (CEA); Dr. SOLLIER, Arnaud (CEA); Dr. OCCELLI, Florent (CEA); Ms. TORCHIO, Raffaella (ESRF); Dr. LOUBEYRE, Paul (CEA)

Recent experimental investigations of deuterium at warm dense matter conditions

The hydrogen isotopes have long provided challenges for both experimental and theoretical investigation of states of warm dense matter. I will review three recent experimental investigations of compressed states of deuterium ranging in pressure from 0.1 TPa to ≈10 TPa, and densities from 0.7 g/cm3 to more than 5 g/cm3.
The first experiment on the National Ignition Facility (NIF) focused on reverberation compression to follow a compression path through the insulator-metal (IM) transition, at temperatures below 2000 K. From optical velocimetry data we inferred the compression path and a jump in optical reflectivity identified the IM transition. A similar experiment at the Z facility identified the transition at a much higher pressure. We have proposed a new interpretation consistent with both experimental results.
The second experiment examined the principal Hugoniot of deuterium up to 550 GPa and reflected-shock states up to 1 TPa. These states are well within the warm dense matter domain: strongly-coupled and partially-degenerate, with temperatures from a few eV to 10 eV. The Hugoniot data are about 4% softer than current first principles models, while the reflected-shock data reach densities about 7% higher than predicted by all models. These discrepancies are large enough, and the data accurate enough, to motivate further investigations of first principles models at these states.
Finally, the compression path of DT fuel in inertial confinement fusion (ICF) follows isentropes to very high density, where little experimental compression data exist. We have developed an experimental platform to compress deuterium along isentropes similar to the ICF paths on the NIF, diagnosing the density using a radiographic technique. Our approach, combining spherical geometry with multi-shock reverberation, can achieve near isentropic compression to multi-TPa pressures. Our initial results have investigated compression to pressures approaching 10 TPa. I will discuss prospects for future developments.

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Primary author(s): P.M. Celliers (Lawrence Livermore National Laboratory)

The classical molecular dynamics at the service of experiments

The fabulous increase of computers capabilities offers an interesting opportunity to directly compare experiments and simulations at the atomic scale. Due to the usual size of experimental samples, only classical approaches can obviously be considered. Moreover, if the external solicitation is highly dynamic (shock, short laser pulse), the dynamic aspects of the sample response cannot be neglected.
Thus, to simulate this type of experiments, we have chosen the method of classical molecular dynamics (MD). In this talk, we will first briefly introduce the MD software developed and used at CEA (the ExaStamp code). Then, two examples will be presented: the fusion of ultra-thin gold samples and Tin phase changes under shock. In these two cases, we will insist (i) on the global hydrodynamic response of the targets, often essential for the understanding of the experimental observations and (ii) on the great importance of the size effects in the simulations: a very large number of atoms can to be required.

Primary author(s) : L. Soulard (CEA, DAM, DIF)

Femtosecond laser-produced periodic plasma in a colloidal crystal probed by XFEL radiation

Studies of materials under high pressures of one Mbar and above is highly relevant for the physics of shock-compressed planetary formation, warm dense matter, and different types of plasma-matter interactions. A unique form of matter such as periodic plasma can be created, for example, by the IR laser interaction with the colloidal crystals made of polystyrene. Extreme pressure and temperature of created plasma lead to the generation of an expanding shock wave that causes compression of the surrounding material. An evolution of periodic plasma obtained from polystyrene colloidal crystals was studied with picosecond time resolution in pump-probe experiments at X-ray free-electron laser LCLS. X-ray Bragg peak parameters were analyzed as a function of time. Simulations of the femtosecond laser-produced plasma in the colloidal crystal were performed. Based on obtained plasma parameters shock wave propagation through the colloidal crystal was simulated and the results are in a good agreement with the experimental data.

Primary author(s) : Ms. MUKHARAMOVA, Nastasia (DESY)
Co-author(s) : Prof. VARTANIANTS, Ivan (DESY); Dr. SERGEY, Lazarev (DESY)

X-ray diffraction of warm dense matter on the Z-accelerator

Experiments on the Sandia Z-accelerator have demonstrated the ability to produce warm dense matter states with unprecedented uniformity, duration, and size, which are ideal for investigations of fundamental material properties. X-ray diffraction (XRD) is a key material science measurement since it provides direct observation of the compression and strain of the crystal lattice, and is used to detect and identify phase transitions. Because of the low signal levels of XRD and due to the destructive nature of Z-Dynamic Materials Properties (DMP) experiments, it is very challenging to detect the XRD pattern close to the Z-DMP load and recover the data. Instead, a new Spherical Crystal Diffraction Imager (SCDI) diagnostic has been developed to relay the diffracted x-rays away from the load debris field.
The SCDI diagnostic utilizes the Z-Beamlet laser to generate 6.2-keV Mn Hea x-rays to probe a shock-compressed sample on the Z-DMP load. A spherically bent crystal composed of highly oriented pyrolytic graphite (HOPG) is used to collect and focus the diffracted x-rays into a 1-inch thick tungsten housing, where an image plate is used to record the data.

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Primary author(s) : Dr. AO, Tommy (Sandia National Laboratories)
Co-author(s) : Dr. SCHOLLMEIER, Marius (Sandia National Laboratories); Dr. KALITA, Patricia (Sandia National Laboratories); Mr. GARD, Paul (Sandia National Laboratories); Mr. WILLIAMS, James (Sandia National Laboratories); Ms. BLADA, Caroline (Sandia National Laboratories); Dr. HANSHAW, Heath (Sandia National Laboratories); Dr. SMITH, Ian (Sandia National Laboratories); Mr. SHORES, Jonathon (Sandia National Laboratories); Mr. SPEAS, Christopher (Sandia National Laboratories); Dr. SEAGLE, Christopher (Sandia National Laboratories)

Dynamics of the Electrical Conductivity and Structure of Warm Dense Aluminum Studied by Single - Shot Terahertz Spectroscopy and Ultrafast Electron Diffraction

Understanding the properties of Warm Dense Matter (WDM) is important for many areas of physics including planetary astrophysics and fusion ignition. Knowledge of the electrical conductivity of WDM is vital for developing accurate models of planetary formation, inertial confinement fusion, and Z-pinches [1]. Aluminum (Al) is as a model system for investigating WDM, and has been studied extensively in theory and experiment. Here we present measurements of the electrical conductivity and structure of laser generated Warm Dense Al (WD-Al). Our experiments used 40 nm free-standing foils pumped into the WDM state with an intense femtosecond laser.
To study the complex-valued electrical conductivity, we used single-shot terahertz timedomain spectroscopy [2]. Terahertz (THz) pulses are ideal probes of conductivity. The relatively long temporal period (˜1 picosecond) compared to the relevant interaction timescales (˜0.03 picosecond) [3] makes THz field s essentially static . Consequently, p roperties measured by THz pulses are very close to the DC properties. From the measured THz transmission , w e determined that the conductivity as low as 1x10ˆ6 S/m depending on the conditions of the WD-Al.
To understand the structure, we used single-shot mega-electron-volt ultrafast electron diffraction (MeV-UED)[4, 5]. MeV-UED is a n ideally suited to probe of the structure of thin films because of the high sc attering cross section , short wavelength , and sub-picosecond pulse duratio n of relativistic electron bunches. Here, we use MeV-UED to study the structural dynamics following intense femtosecond laser irradiation. These measuremen ts provide crucial characte rization of the state and density of the WD-Al probed by the THz pulse , as well as the timescale of melting of Al films at high excitation densities.

Primary author(s) : Dr. OFORI-OKAI, Benjamin K. (SLAC)

Electron kinetics induced by X-ray FEL excitation of Au

Electron kinetics in strongly out-of-equilibrium states is an uncharted frontier in Warm Dense Matter science. Apart from its fundamental significance, electron kinetics plays a key role in determining the properties of ultrafast heated solids prior to the thermalization of the electron subsystem. This is of particular interest to the growing studies of Warm Dense Mater produced with intense lasers and FELs.
Here we report on the studies of electron kinetics in thin layer of WDM gold produced with 245 eV X-ray pulses at the FEL facility FLASH in Hamburg. Experimental findings and challenges for understanding and modeling the complex relaxation processes following X-ray excitation in Au are discussed.

Primary author(s) : B. Ziaja (1,6)
Co-author(s) : Z. Chen (2), P. Hering (2), M.Z. Mo (2), C. Curry (1,2), B. Russell (1,2), J. Kim (2), S. Brown (2), S. Glenzer (2), S. Tolekis (1), N. Borches (3), M. Buescher (3), T. Takanori (1), H. Hoeppner (1), A. Grolleau (4), Y. Tsui (5), V. Saxena (1), N. Medvedev (1) , P. Piekarz (6), V. Recoules (7), B. Rethfeld (8), D. Gericke (9), and A. Ng (10)

(1) DESY, Germany
(2) SLAC, U.S.A.
(3) University of Oldenburg, Germany
(4) Universite de Bordeaux, France
(5) University of Alberta, Canada
(6) Institute of Nuclear Physics, PAS, Poland
(7) CEA, DAM, DIF, F-91297 Arpajon, France
(8) Technical University of Kaiserslautern, Germany
(9) University of Warwick, U.K.
(10) University of British Columbia, Canada

Emission wavelength control in hard x-ray lasers with Bragg crystal target

We demonstrated the solid material pumped by intense resonant hard x-ray can be used for high gain medium for inner shell transition lasers. We have succeeded K-alpha (1s-2p) inner shell ionized laser of Cu atoms, which has 0.15nm wavelength an 8keV photon energy. In this laser transition, the gain band width have 3˜5eV in 8040 eV emission center. To consider the emission life time would be about 1fs, which is decided by the life time of the corresponding states, the band width of single frequency laser should be down to about 2eV or less. One of idea to control emission band width is external seeding. We already demonstrated this with two color operation of SACLA XFEL, in which one color is tuned to the pumped photon energy and the other color is tuned to the seed photon energy of 1s-2p transition. In this method, intense resonant light can be initiated and that control the emission process of the atoms. However, there is still large difference to compare the usual optical lasers. One of the biggest difference is there is no cavity control method in the hard x-ray lasers. Normally, that cavity for hard x ray is very difficult. Here, we propose a new type of hard x-ray lasers, which is similar mechanism of the emission control of cavity lasers. In this proposal laser, crystal of Bragg resonance condition is used for achieving the standing wave. The crystal angle is adjusted that the lattice spacing of the normal surfaces is matched to the wavelength of the K-shell laser. By this scheme, we demonstrate spatial mode controlled laser, cavity controlled emission wavelength laser, and anti-resonance lasers. Again, in hard x-ray laser, it is very difficult to prepare the good mirror for cavity. Therefore, this Bragg standing wave lasers will be useful to achieve hard x-ray laser with cavity type controlled method.

Primary author(s) : Prof. YONEDA, Hitoki (Institute for Laser Science)

Ultrafast Anisotropic Disordering in X-ray Heated Graphite

By using X-ray Free Electron Lasers (XFELs), samples can be driven to high energy density (HED) states through direct hard X-ray irradiation. As a heating method, this offers advantages, as a fast, isochoric and volumetric drive [1]. However, because it proceeds mostly by exciting high-energy photo- and Auger electrons, it is complex to model, and tends to heat a much larger region of the sample than the irradiated spot [2].
In this talk, I will present results from the Japanese XFEL SACLA (SPRing-8 Angstrom Compact free electron LAser). Using its two-colour split and delay mode, the first pulse irradiated graphite samples with incident X-ray intensities on the order of 10ˆ20 W/cm2, with the second pulse probing changes in the atomic structure by diffraction [3]. Within 10s of femtoseconds, there is a significant loss of signal in diffraction peaks with interplanar correlations, while the signal from in-plane correlations increases. We believe that this is due to the breaking of the weaker bonds between planes [4], and a possible relocation of electrons into the covalent in-plane bonds – an effect similar to bond hardening [5].

References [1] Medvedev & Ziaja, Sci. Rep. 8 (2018). [2] Grum-Grzhimailo et al., EPJ D 71 (2017). [3] Inoue et al., PNAS 113 (2016). [4] Jeschke et al., PRL 87 (2001). [5] Ernstorfer et al., Science 323 (2009).

Primary author(s) : Dr. HARTLEY, Nicholas (HZDR)
Co-author(s) : Dr. HUANG, Lingen (HZDR); Dr. INUBISHI, Yuichi (SPRing-8); Mr. KAMIMURA, Nobuki (Osaka University); Mr. KATAGIRI, Kento (Osaka University); Dr. KON, Akira (SPRing-8); Dr. MAKITA, Mikako (European XFEL); Dr. MATSUOKA, Takeshi (Osaka University); Dr. LU, Wei (European XFEL); Dr. MEDVEDEV, Nikita (FZU); Mr. NAKAJIMA, Shogo (Osaka University); Dr. PIKUZ, Tatiana (Osaka University); Dr. RODE, Andrei (ANU); Ms. ROHATSCH, Katja (HZDR); Mr. SAGAE, Daisuke (Osaka University); Ms. SCHUSTER, Anja (HZDR); Dr. TONO, Kensuke (SPRing-8); Dr. VORBERGER, Jan (HZDR); Dr. YABUUCHI, Toshinori (SPRing-8); Dr. OZAKI, Norimasa (Osaka University); Dr. KRAUS, Dominik (HZDR)

Energy relaxation and electron phonon coupling in laser heated solids

Laser irradiation of metals can heat the electrons to high energies within femtoseconds. The electrons transfer this gained energy onto the lattice via electron phonon coupling. This process is analysed via linear response calculations within a density functional theory framework. Several elements and materials are studied and the electron-phonon relaxation time is compared to phonon-phonon coupling. The applicability of simple two-temperature relaxation models is tested on the basis of DFT calculations as well as via experiment.
We also analyse the possibility of non-equilibrium electron populations, as for instance in ferromagnetic materials. The Transition to energy relaxation in (fluid) warm dense matter is discussed.

Primary author(s) : Dr. VORBERGER, Jan (HZDR)

Development of the National Ignition Facility ramp compression platform and the use of ramp compression experiments in construction of material models

It is important to a number of fields to be able to accurately simulate processes and material responses under extreme conditions. Using sophisticated hydrodynamic codes, we can model giant impacts, planetary formation, and inertial confinement fusion implosions. The degree to which these simulations reflect reality, however, is dependent on how well we understand the materials and physics involved. We need material models that both agree with experimental data and also reflect the accuracy with which our measurements are made. In the first part of this presentation, I will present an overview of the extreme conditions we can experimentally probe using the NIF ramp compression platform, including highlighting recent results on copper compressed to 2400 GPa. In the second part I will discuss a framework for using both our experimental measurements and the associated experimental uncertainties to construct equation of state models that reflect not just our current best measurements, but also the accuracy of those measurements.

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Primary author(s) : Dr. Ali, Suzanne (Lawrence Livermore National Laboratory)

Paramagnetic-to-diamagnetic transition in dense liquid iron and its influence on electronic transport properties

The electronic transport properties of warm dense liquid iron are important properties for understanding the magnetic field generation in Earth-like and other solid planets. Here we investigate the electrical and thermal conductivity with spin-polarized density-functionaltheory-based simulations over a significant pressure and temperature range using the Kubo-Greenwood formalism. We find that a paramagnetic state is stable in the liquid up to high temperatures at ambient pressure. It is shown that the overestimation of results from exploding wire experiments by more than 30% that occurs in spin-degenerate simulations is reduced to 10% or less when spin polarization is taken into account. Direct comparisons between spin-polarized and spin-degenerate simulations reveal that the spin effects on the conductivities enter via changes in both ionic and electronic structure. Along the 3700 K isotherm, we explore the persistence of magnetic fluctuations toward high densities, and beyond 20-50 GPa the liquid becomes diamagnetic, which suggests the existence of a continuous paramagnetic-to-diamagnetic transition. This transition exerts a significant influence on the transport properties of liquid iron and is potentially of high relevance for dynamo processes in Mercury and Mars. This work is supported by the DFG within the FOR 2440 “Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics.”

Primary author(s) : Dr. FRENCH, Martin (Universität Rostock)
Co-author(s) : KORELL, Jean-alexander (Universität Rostock); STEINLE-NEUMANN, Gerd (Bayerisches Geoinstitut); Prof. REDMER, Ronald (Universität Rostock)

Charged Particle Stopping Power of Nonideal Plasmas

The deceleration of energetic charged particles is one of the prominent processes allowing to study and diagnose the behaviour of dense plasmas and warm dense matter. Recently, a number of experiments were able to cover parameter regions previously not covered. Thus, theoretical models can now be tested on a firmer basis and, indeed, few experiments could clearly distinguish between different models. As a results, a number of common and easy-touse models were shown to be inapplicable in the region of strong interactions between the beam ions and the plasma as well as for very hot temperatures related to inertial confinement
fusion.
This contribution will focus on the kinetic theory approach to the stopping power and discuss the different approximation schemes developed so far. On this basis, results that clearly show signs of deviations from the common models are presented. In the next step, two recent experiments are briefly reviewed and their results are compared to the models presented before. The comparison shows that only models that treat the interactions of beam and plasma particles nonperturbatively agree with data for intermediate beam velocities. Moreover, we need a quantum description for very hot plasmas occurring in ICF experiments as quantum diffraction is important here. Unfortunately, the very interesting region of strongly coupled and degenerate plasmas has neither be covered by experiments nor, in full, by theory yet. This contribution will conclude by drafting an approach that will resolve the problems related to a combination of strong interactions and quantum degeneracy.

Primary author(s) : Dr. GERICKE, Dirk (University of Warwick)

Characterizing the Ionization Potential Depression in Dense Carbon Plasmas with High-Precision Spectrally Resolved X-ray Scattering

We show the possibility of obtaining highly precise measurements of the ionization potential depression in dense plasmas with spectrally resolved X-ray scattering, while simultaneously determining the electron temperature and the free electron density. A proof-of-principle experiment at the Linac Coherent Light Source [1], probing isochorically heated carbon samples, demonstrates the capabilities of this method. Following these restuls, planned precision experiments to be performed at the HED instrument of European XFEL will be discussed.

[1] D. Kraus et al., Plasma Phys. Contr. Fusion 61, 014015 (2019)

Primary author(s) : Dr. KRAUS, Dominik (HZDR)

Posters:

(sorted according to submission time)

1 Bailie, David, Queen's U. Belfast, *'K-edge shift under warm dense matter conditions'*

2 Brouwer, Nils, CEA DAM DIF, *'Spin-Orbit effects in optical and XANES spectra of warm dense copper and gold'*

3 Hou, Yong, NUDT, *'Core-hole screening influences on shift of near-threshold orbitals in warm dense Au matter'*

4 Hyland, Cormac, Queen's U. Belfast, '*Measurement of Free-free Absorption of XUV Radiation in Warm Dense Aluminium'*

5 Pan, Xiayun, HZDR, '*X-ray Crystal Spectrometers for Temperature Measurement of Laser-heated Dense Plasmas'*

6 Zeng, Jiaolong, NUDT, *'PhD'*

7 Zhang, Shen, NUDT, *'Link between K absorption edges and thermodynamic properties of warm dense aluminum established by first-principles calculations'*

8 Baczewski , Andrew, Sandia NL, '*Transport properties of magnetized warm dense matter using time-dependent density functional theory'*

9 Lee, Jong-Won, GIST, '*Femtosecond measurement of electron-hole equilibration in warm dense copper'*

10 Mukharamova, Nastasia, DESY, '*Femtosecond laser-produced periodic plasma in a colloidal crystal probed by XFEL radiation'*

11 Perez-Martin, Pablo, HZDR, *'Investigation of thermodynamic properties of non-equilibrium dense matter states with enhanced x-ray Thomson scattering'*

12 Smirnov, Nikolai, RFNC, *'Thermodynamic properties of tantalum under non-equilibrum heating from first-principles calculations'*

13 Apfelbaum, Evgeny, JIHT, '*The calculations of thermophysical properties of low temperature Pb plasma'*

14 Cebulla, Daniel, U. Rostock, *'DFT+U equation of state for iron oxide'*

15 Dorchies, Fabien, CELIA, '*Experimental investigation of the electron structure dynamics in non-equilibrium warm dense copper'*

16 French, Martin, U. Rostock, *'Thermal conductivity of water plasmas from ab initio simulations'*

17 Groth, Simon, U. Kiel, ' *Ab initio Reconstruction of the Dynamic Structure Factor of the Uniform Electron Gas'*

18 Li, Qiong, IAPCM, ' *The electrical conductivity of metal plasma'*

19 Liu, Haifeng, IAPCM, *'Equation of state in wide regime for Hydrogen: Construction and Validation'*

20 Liu, Dongxiao, RCLF, CAEP, *'Reflectivity evolution of warm dense gold in metal-nonmetal transition regime'*

21 Marizy, Adrien, CEA DAM, *'Microsecond joule heatings of metal foils: EOS, electrical resistivity and EDXAS measurements in the warm dense matter regime'*

22 Migdal, Kirill, Dukhov RIA, '*Radiation damage caused by fast charged particles: implementation of effective force field method'*

23 Rightley, Shane, U. Iowa, *'A New Model for Collisional Transport in Warm Dense Plasmas'*

24 Rykounov, Alexey, RFNC, '*Thermodynamic properties of C-N-O-H mixture in the region of non-ideal plasma'*

25 Saitov, Ilnur, JIHT RAS, *'Ab initio simulation of formation of conducting solid and fluid hydrogen under high pressures'*

26 Sartan, Roman, JIHT RAS, '*Equation of state of warm dense hydrogen in the region of metastability'*

27 Wang, Yufeng, IFP, '*Numerical simulation of coupled air plasma after strong shock based on the thermodynamic chemical model'*

28 Zhang, Dongwen, NUDT, *'Preliminary study on conductivity of warm-dense matter in terahertz range'*

29 Bethkenhagen, Mandy, U. Rostock, *'Large-scale O(N) DFT calculations for carbon at high temperature'*

30 Smid, Michal, HZDR, '*Laser wakefield accelerated betatron beam used for ultrafast Warm Dense Matter studies'*

31 Tahir, Naeem, GSI, '*High Energy Density Physics Research at the Facility for Antiprotons and Ion Research [FAIR] at Darmstadt'*

32 Torchio, Raffaella, ESRF, *'The High Power Laser Facility at the ESRF'*

33 Zapolnova, Ekaterina, DESY, *'XUV plasma switch for THz: new temporal overlap tool for XUV-THz pump-probe experiments at FELs'*

34 Banjafar, Mohammadreza, EUXFEL, *'Grazing-incidence x-ray scattering of surfaces upon high-intensity laser irradiation'*