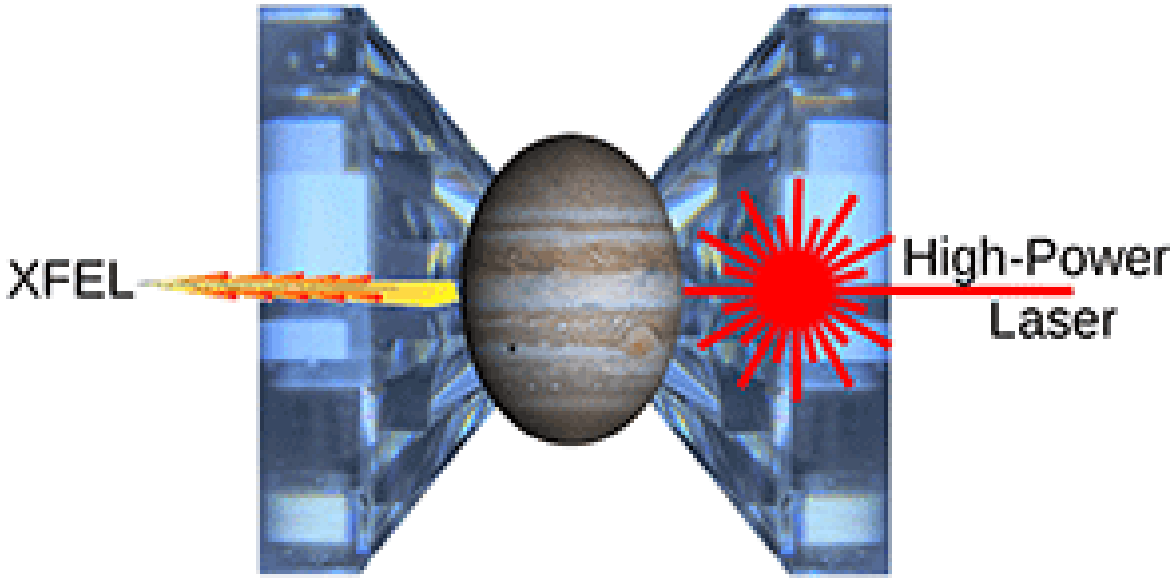

5th Joint Workshop on High Pressure, Planetary and Plasma Physics (5thHP4)

September 14th noon – September 16th noon
DESY & European XFEL, Hamburg

Introduction:

The generation and diagnostics of extreme states of matter as appearing in the interior of planets, brown dwarfs and stars is one of the key scientific challenges in a number of scientific fields. These include:

- Generation of such conditions at FLASH and the future free electron laser facility (European XFEL).
- Generation of higher pressures in static experiments both in the laboratory and at synchrotron facilities (PETRA III).
- Development of new diagnostic tools.
- Predictions of high pressure and temperature properties of materials from ab-initio methods.
- Application of such results to the study of interior of planetary and astrophysical bodies.

To bring together researchers from these different fields in the physical sciences a workshop series has been established by DESY, XFEL GmbH, DLR Berlin, the University of Rostock and Bayerisches Goinstitut to discuss related topics and problems. Earlier workshops were held at DESY Hamburg (2012), DLR Berlin (2013), University of Rostock (2014) and the Bayerisches Geoinstitut at the University of Bayreuth.

The aim of the upcoming workshop is to continue the discussion of scientific questions with relevance for extreme planetary environments in terms of high pressure (HP) and high temperature (HT). The conditions prevalent in the deep interiors and atmospheric envelopes of solar system planets, their satellites as well as massive solid and gas giant extrasolar planets, respectively, and are not fully accessible by conventional experimental and theoretical methods. New and enabling techniques to be used in the HP/HT regime are based on the combination of intense pulsed x-ray sources with pulsed sample excitation, in particular but not exclusively related to high energy optical lasers. Simultaneously, ab initio simulations for matter under extreme conditions provide a more and more predictive data set for planetary interiors in this HP/HT regime.

The following topics will be part of the workshop:

- Evolution and structure of giant planet interiors
- Interior structure, bulk composition, and internal geodynamics of solid planets
- Deep volatile cycles and exchange processes between geochemical reservoirs
- Physics and chemistry of impact processes
- Equations of state, petrology, and geochemistry of planetary materials
- Melting relations and phase transformations of materials at extreme states
- Dynamic and ultrafast processes in strongly excited solids or similar,
- Compression experiments using high-power optical and free electron lasers
- Laboratory experiments using multi-anvil and diamond-anvil cells
- Ab-initio simulation studies for matter under extreme conditions

Final Schedule

Wednesday September 14th		
12:00 – 13:20	Light Lunch in the foyer of the Flash Hall and Registration	
13:20 – 13:30	**Welcome**	U. Zastrau & H. P. Liermann
Session 1: Hydrogen and Helium *Chair: U. Zastrau*		
13:30 – 14:10	Dynamic compression experiments on deuterium and their implications for first-principles theory (invited)	M. Knudson (SNL)
14:10 – 14:50	Investigating the Hydrogen Plasma Phase Transition on the National Ignition Facility (invited)	M. Millot (LLNL)
14:50 – 15:10	Miscibility gap of hydrogen-helium mixtures	M. Schöttler (Uni. Rostock)
15:10 – 15:50	Coffee Break	
Session 2: Giant planets *Chair: R. Redmer*		
15:50 – 16:30	Exploring Jupiter's interior before Juno (invited)	Y. Miguel (Obser. Cote d'Azur)
16:30 – 16:50	X-ray diffraction of water dynamically compressed to 4 Mbar and evidence for a new crystalline ice phase	F. Coppari (LLNL)
16:50 – 17:10	A sandwich stable layer in Saturn's deep interior	W. Dietrich (MPI Solar Syst. Res.)
17:10 – 17:30	Predicting Juno's measurements of Jupiter's internal field and secular variation based on numerical dynamo simulations	J. Wicht (MPI Solar Syst. Res.)
18:00 – open	Suggestions for local restaurants / Possibility to join the PETRA III X Inauguration	

Thursday September 15th		
8:45 – 9:00	Coffee, Registration, Announcements	
Session 3: Earth's core *Chair: Steinle-Neumann*		
9:00 – 9:40	Thermal history of Earth's coupled core-mantle system with high core conductivity (invited)	C. Davies (Uni. Leeds)
9:40 – 10:20	Transport properties of iron at Earth's core conditions: a first-principles theory (invited)	S. Simak (Linköping Uni.)
10:20 – 10:50	Coffee Break	
10:50 – 11:10	Direct measurements of thermal conductivity in the Earth's core	Z. Konopkova (European XFEL)
11:10 – 11:30	Melting and phase change for laser-shocked iron	D. Riley (Queen's Uni. Belfast)
Session 4: Rocky mantles *Chair: Z. Konopkova*		
11:30 – 12:10	Ab initio equation of states for planetary and exoplanetary modeling (invited)	S. Mazevet (Université Paris)
12:10 – 13:10	Light Lunch in foyer of the Flash Hall	
13:10 – 13:30	High pressure phase diagram of MgO and FeO	D. Cebulla (Uni. Rostock)
13:30 – 13:50	Decaying shock studies of the MgO and $MgSiO_3$ high pressure phase diagrams and implications for Earth-like and super-Earth planets.	R. Bolis (Ecole Polytechnique)
13:50 – 14:10	A computational framework of mantle thermodynamics	G. Steinle-Neumann (BGI)
14:10 – 14:40	Coffee Break	

Session 5: Phase transitions *Chair: M. McMahon*		
14:40 – 15:20	Structural transitions in shock-compressed hydrocarbons (invited)	D. Kraus (HZDR)
15:20 – 16:00	Ultra-high pressure equation of state using laser compression (invited)	A. Lazicky (LLNL)
16:00 – 16:20	Warm Dense Carbon on XFELs	N. Hartley (HZDR)
16:20 – 16:40	The phase diagram of water under extreme conditions of pressure and temperature	M. French (Uni. Rostock)
16:40 – 19:00	Poster Session with Refreshments	
19:30 – open	BBQ at DESY canteen	

Friday September 16th		
8:45 – 9:00	Coffee, Registration, Announcements	
Session 6: Diagnostics of shocked metals *Chair: U. Zastrau*		
9:00 – 9:40	Structure factor measurements in strongly coupled plasmas in the long wavelength limit (invited)	P. Neumayer (GSI)
9:40 – 10:20	Doing time-resolved synchrotron x-ray measurements at very high pressure: a strategy and first results (invited)	F. Occelli (CEA)
10:20 – 10:40	Ab initio simulations of the dynamic ion structure factor of warm dense lithium	R. Redmer (Uni. Rostock)
10:40 – 11:10	Coffee Break	
Session 7: Metals at HP-HT *Chair: H. P. Liermann*		
11:10 – 11:50	Complex Structures in Shock-Compressed Scandium to 82 GPa (invited)	M. McMahon (Uni. Edinburgh)
11:50 – 12:30	Time resolved x-ray diffraction: dynamics of pressure induced structural phase transition in bismuth (invited)	Z. Jenei (LLNL)
12:30 – 12:50	Time-resolved XANES spectroscopy using a table-top laser-plasma source: study of copper under extreme conditions and out-of-equilibrium	N. Jourdain (CEA)
12:50 – 13:10	Non-Drude conductivities in isochorically heated warm dense aluminum observed by inelastic x-ray scattering	P. Sperling (European XFEL)
13:10 – 13:30	Electronic transport properties of metals at extreme conditions	F. Wagle (BGI)
13:30 – 13:35	Concluding Remarks	U. Zastrau, H. P. Liermann

Book of Abstracts

5th Joint Workshop on High Pressure, Planetary and Plasma Physics (5thHP4)

Session 1: Hydrogen and Helium

Dynamic compression experiments on deuterium and their implications for first-principles theory

M. Knudson[1], M. Desjarlais[1], R. Lemke[1], K. Cochrane[1], M. Savage[1], D. Bliss[1], T. Mattsson[1], R. Redmer[2], A. Becker[2]

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Recently a so-called shock-ramp platform has been developed on the Sandia Z Accelerator to access off-Hugoniot states in liquids. The accelerator delivers a twostep current pulse; the first accelerates the electrode to a reasonably constant velocity, which upon impact with the sample cell creates a well-defined shock, the subsequent current rise produces ramp compression from the initially shocked state. This technique generates relatively cool (~1-2 kK), high pressure (>300 GPa), high compression states (~10-15 fold compression) states, allowing experimental access to the region of phase space where hydrogen is predicted to undergo a first-order phase transition from an insulating molecular-like liquid to a conducting atomic-like liquid. In this talk we will discuss the experimental platform, survey the various theoretical predictions for the liquid-liquid, insulator- to-metal transition in hydrogen, and present the results of experiments that clearly show an abrupt transition to a metallic state. We will also present recent Hugoniot and reshock data for deuterium with unprecedented precision in the vicinity of the molecular-to-atomic transition. These data not only establish maximum compression along the Hugoniot at 4.5-fold, but also enable high-fidelity comparisons with first-principles theory.

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

Investigating the Hydrogen Plasma Phase Transition on the National Ignition Facility

M. Millot[1], P.M. Celliers[1], S. Brygoo[2], J. Eggert[1], R. Jeanloz[3], G. W. Collins[1], R. Hemely[4], A. Goncharov[4], P. Loubeyer[2], S. McWilliams[5], J.R. Rygg[1], S. LePape[1], D. Fratanduono[1], S. Hamel[1], N. Meezan[1], L. Peterson[1], D. Braun[1]

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New dynamic-compression techniques allow scientists to recreate the material states expected to exist in the deep interiors of planets, including the newly discovered extra solar planets. At the conditions existing deep inside stars and planets, pressure produces highly degenerate conditions (strong quantum effects), with atoms brought closer than the Bohr radius. State-of-the art calculations indicate that such strong degeneracy effects induce the insulator conductor transition in fluid hydrogen to become first-order, i.e. discontinuous, at temperatures below about 2500 K. This phase transition is called the Plasma Phase Transition (PPT). This problem challenges the most advanced simulations and theories resulting in a span of proposed conditions for the PPT from 1 to 5 Mbar, between 1000 and 2500 K. At higher temperature the metallization onset is thought to be continuous.

We will present recent experiments using a reverberation compression scheme on the National Ignition Facility to compress cryogenic deuterium up to several megabars (1Mbar=100 GPa) while keeping the temperature much lower than using single shock compression.

This work was performed under the auspices of the U.S. Department of Energy by LLNL under contract DE-AC52-07NA27344.

Miscibility gap of hydrogen-heliummixtures

M. Schöttler R. Redmer

Universität Rostock

Our focus is the calculation of a demixing phase diagram of hydrogen-helium mixtures for application in planetary and astrophysics. Hydrogen-helium demixing has been proposed as a possible source of Saturn's excess luminosity: When the planetary isentrope enters the demixing region, helium-rich droplets can form and sink toward the planet's core, thus, acting as an additional source of heat.

Demixing is calculated by computing the free enthalpy G(x,p,T) at constant pressure p and temperature T for different helium fractions x. We use finite-temperature density functional theory molecular dynamic simulations to obtain the equation of state for given volumes and temperatures.

The choice of an exchange-correlation (XC) functional, that captures the relevant physics, is of high importance. It has been shown that standard approximations lack the ability to adequately describe the hydrogen metallization, which is directly connected to the H-He demixing. Functionals, that take non-local correlations into account, e.g., vdW-DF [Dion et al., PRL 92, 246401 (2004)], are in better agreement with experiments [Knudson et al., Science 348, 1455 (2015)]. Benchmarking studies with many XC functionals against QMC calculations suggest vdW-DF as an appropriate functional also for hydrogen-helium mixtures [Clay et al., PRB 89, 184106 (2014)]. Here, we present a demixing phase diagram of H-He mixtures calculated with vdW-DF and compare with previous calculations derived with the PBE functional [Lorenzen et al.,PRL 102, 115701 (2009)]. Differences and implications for planetary physics are discussed.

Session 2: Giant planets

Exploring Jupiter’s interior before Juno

Y. Miguel

Observatoire de la Cote d'Azur

Jupiter is key to understand the origin of our Solar system. It was one of the first planets to form and saved in its interior valuable information about the physics and chemistry of the primitive nebula. Nevertheless, the distribution and amount of heavy elements in its interior is difficult to constrain and degeneracies arise depending on assumed observational constrains and model parameters in interior structure calculations.

Juno will provide new observational constrains for the interior of the planet helping to understand Jupiter’s interior. We will show that one of the big challenges in deriving a core mass and a global composition of the planet still rests on the accuracy of equations of state that can be used. Resolving these will greatly help the interpretation of Juno data.

X-ray diffraction of water dynamically compressed to 4 Mbar and evidence for a new crystalline ice phase

F. Coppari, M. Millot, R. Rygg, A. Correa Barrios, J. Eggert

Lawrence Livermore National Laboratory

The study of water at extreme conditions is important for planetary science, water being thought to dominate the interiors of Neptune, Uranus and extrasolar mini-Neptunes. At the extreme conditions deep inside these bodies water has been predicted to become superionic with a solid lattice of oxygen and diffusing hydrogen. Optical measurements[1] combined with previous electrical conductivity experiments[2] reveal high ionic electrical conduction near 1.5 Mbar and 4000 K, consistent with the predictions for superionicity. However, no direct experimental evidence exists so far documenting a solid oxygen lattice at these conditions.

Nano-second x-ray diffraction measurements of matter dynamically compressed to multimegabar pressures are now routinely collected at the Omega laser facility [3,4,5]. However extending the technique to measure diffraction of low-Z solids remains extremely challenging. It requires optimization of the laser drive pulse shape (to follow a low-entropy compression path) and maximization of the signal to-background. Here we present diffraction data on water dynamically compressed into dense ice. A specifically designed stack of laser pulses was used to compress liquid water through small shocks. The laser power was tuned to follow the pressure-temperature compression path to explore conditions approaching Neptune's core mantle boundary near 4 Mbar and 5000-6000 K.

The new data evidence a solid oxygen lattice demonstrating that we succeeded in compressing water into crystalline dense ice. Our data suggest the existence of a temperature-driven solid-solid phase transition in the predicted stability domain of superionic water ice and they indicate that water melting temperature increases quickly above 70 GPa and might exceed the interior temperature of large icy planets. Therefore the stability of a new crystalline phase of water at extreme conditions has broad implications for planetary science[6].

Performed under Contract No. DE-AC52-07NA27344.

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A sandwich stable layer in Saturn's deep interior

W. Dietrich[1], J. Wicht[1], T. Gastine[2]

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The observation of Saturn's magnetic field and surface winds challenged interior models for decades. The magnetic field is much more axisymmetric than simpler 3D MHD models typically reproduce. The surface winds inferred by cloud tracking show a strong equatorial prograde (eastwards) jet and several much weaker jets closer to the poles. Both features might be explained by a sandwiched stably stratified layer (S3L) between a deeper convective dynamo and a shallower turbulent convective, but nonmagnetic region. Such a layer will then axisymmetrise the dynamo-generated magnetic field and alter the surface manisfestation of the differential rotation, e.g. creating numerous high-latitude jets.

Saturn's atmosphere consists mainly of helium and hydrogen. Both are thought to be well mixed by rapid convective flows in the outer convective region, where hydrogen is molecular. However, at greater depth (r/r_S = 0.65, or at 1Mbar) hydrogen becomes metallic and immiscible with helium. Helium then rains out and sinks downwards. At even greater depth, the temperature and helium abundance are much higher such that helium and hydrogen are miscible again (immiscibility gap). This will lead to a helium-depleted outer and a helium-enriched inner convective zone. In between a strong helium gradient establishes and defines a compositional stable stratification suppressing convection, magnetic field generation and differential rotation.

We therefore numerically model the effect of a S3L on convection and the generation of differential rotation. The S3L is implemented by defining a background entropy profile. Our results suggest, that the S3L efficiently damps the convection, the resulting differential rotation and leads to a more Saturn-like surface zonal flow profile. However, the emerging equatorial prograde reaches up to the upper edge of the S3L and is hence in comparison to the observations too broad. If the equatorial deep-reaching prograde jet is always bounded by the S3L, our results are indicative of a shallower de-mixing or metallisation depth.

Predicting possible Juno's internal field and secular variation models based on numerical dynamo simulations

J. Wicht[1], R. Holme[2], L. Durate[3], T. Gastine[4]

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With Juno orbiting Jupiter, new insights on the planet's magnetic field and interior structure can be expected within the next months. We conduct numerical simulations of the internal dynamo process to help interpreting the measurements. The simulations were performed with the MHD code MagIC and explore various parameter combinations as well as different internal density and electrical conductivity profiles. Surface magnetic fields closely resemble known magnetic field models when the convective driving is intermediate. Weak driving yields too simplistic field geometries while strong driving promotes multipolar rather than dipole dominated magnetic fields. The combination of strong background density stratification and an electrical conductivity profile that incorporates the weakly conducting outer molecular hydrogen layer is another important ingredient of Jupiter-like dipole dominated dynamos. While details of the density profile hardly matter, the specific form of the electrical conductivity profile determines the depth of the dynamo region and thus influences the relative importance of the magnetic dipole (magnetic spectrum).

The convective flow is dominated by a realistic prograde equatorial jet but lacks multiple mid to high latitude jets which, according to our simulations, seem incompatible with a Jupiter like magnetic field. Using the Juno mission trajectory and assuming an isotropic measurement error of 100 nT we could recover our numerical model fields to spherical harmonic degree 18, and secular variation (SV) perhaps to degree 5. The field shows characteristic bands where the equatorial jet reaches down to higher conductivities and promotes a secondary local dynamo effect. The presence of these bands as well as the SV caused by zonal flow advection may offer important clues on the depth of the zonal jets. The form of the spectrum can provide additional information on the general depth of the dynamo region: The numerical simulations suggest that dynamo action starts at the radius where the magnetic Reynolds number, the ratio of Ohmic dissipation time to convective turnover time, exceeds about 50. This roughly agrees with the depth where the magnetic power spectrum is white for spherical harmonics degrees beyond four.

Session 3: Earth's core

Thermal history of Earth's coupled core-mantle system with high core conductivity

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Paleomagnetic observations that indicate a geodynamo as old as 4.2 Gyr are at odds with the "new core paradox", which claims insufficient energy to drive the ancient geodynamo prior to inner core nucleation. Recent upward revisions to the thermal conductivity of iron in the core strain the energy budget by increasing the conductive heat flow that must be overcome in order to drive thermal convection and maintain an ancient geodynamo. We address this paradox by computing thermal-magnetic evolutions of the Earth using a 1-D model with parameterizations for heat sources and sinks in the mantle and core. This model includes a number of important new features that have not been previous coupled in a single model. New features in the mantle model include enhanced mantle heat loss to due extrusive volcanism, crust formation and insolation, and latent heating due to magma ocean solidification. New features in the core model include realistic iron conductivities, time-dependent partitioning of light elements (O, S, and Si) between solid and liquid and their effect on the liquidus depression and gravitational energy release. Core evolutions derived from an energy model are compared to an energy-entropy model, which accounts for ohmic dissipation. We identify the conditions necessary to avoid shut-down of the geodynamo prior to inner core nucleation and to maintain a strong magnetic field over the last 4.2 Gyr. Using a dipole field scaling law derived from numerical dynamo models we compare the predicted paleo-dipole intensity to the paleointensity record and speculate on possible observational evidence for the inner core nucleation event.

Transport properties of iron at Earth's core conditions: a first-principles theory

S. Simak

IFM, Linköping University

Transport properties of iron at high temperatures and pressures are of obvious importance to geophysics. Combining the density functional and dynamical mean field theories we study the impact of electron correlations on electrical and thermal resistivity of hexagonal close-packed Fe at Earth's core conditions. We show that it behaves as a nearly perfect Fermi liquid. The quadratic dependence of the scattering rate in Fermi liquids leads to a modification of the Wiedemann-Franz law with suppression of the thermal conductivity as compared to the electrical one. This significantly increases the electron-electron thermal resistivity which is found to be of comparable magnitude to the electron-phonon one.

Direct measurements of thermal conductivity in the Earth's core

Z. Konôpková[1], R. S. McWilliams[2], N. Gomez-Perez[2], A. Goncharov[3]

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The transport properties of minerals and fluids control the flow of thermal energy inside the Earth and other planets, ruling over their internal dynamics and evolution. In the Earth's core, the thermal conductivity of iron alloys defines the adiabatic heat flux and thus, the energy available to support geodynamo (Nimmo, 2015). Recently, a 'core paradox' (Olson, 2013) emerged as a consequence of high thermal conductivity of the core material as proposed from recent theoretical studies at high temperatures (de Koker et al., 2012 and Pozzo et al., 2012) and experimental electrical resistivity measurements at ambient temperatures (Gomi et al., 2013). Under such circumstances, evidence of an ancient magnetic field is difficult to reconcile with the high energy fluxes required by the high thermal conductivity values. Alternative scenarios for the dynamics, driving forces, and thermal structure in the outer core that can produce Earth's magnetic field have been proposed, but problems still remain (e.g. Hirose et al., 2013). In this study, we used a modified flash heating measurement of thermal conductivity, applied to a pre-heated compressed iron foil in the diamond anvil cell, and directly determined the thermal conductivity of iron up to planetary core temperatures and pressures. Our measurements place the thermal conductivity of Earth core material near the lower end of previous estimates, at 18-44 W/m/K. The results are in agreement with core thermal conductivity estimates based on the electrical resistivity behavior of iron at high pressure and temperature by Stacey and Loper (2007) and Seagle et al. (2013) and mitigate the thermal transport problem in Earth's core.

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Melting and phase change for laser-shocked iron

S. White[1], B. Kettle[1], C. L. S. Lewis[1] and D. Riley[1], S. H. Glenzer[2], E. Gamboa[2], B. Nagler[2] H. J. Lee[2], C. D. Murphy[3] D. O. Gericke[4] J. Vorberger[5]

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Using the LCLS facility at the SLAC National Accelerator Centre, we have observed X-ray scattering from samples of Fe that have been compressed with laser driven shocks with pressure exceeding 300GPa. Comparison of the observed scattering for melted samples with modelling with a hypernetted chain model and DFT molecular dynamics indicates that a strong short range repulsive term is present in the inter-ionic potential. For shots where melting is incomplete or only partially achieved and we observe evidence of hexagonal close packed crystal structure but no clear evidence of a double-hexagonal close packed structure.

Session 4: Rocky mantles

Ab initio equation of states for planetary and exoplanetary modeling

S. Mazevet[1,3], T. Tsuchiya[2], R. Musella[1], J. Bouchet[3], V. Recoules[3], F. Guyot[4], G. Morard[4], A. Benuzzi-Mounaix[5,1], A. Licari[6], F. Soubiran[6], G. Chabrier[6]

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Using ab initio molecular dynamics simulations, we recently calculated equations of state for the main constituents of planetary interiors: H, He, H_2O, $MgSiO_3$ (MgO,SiO_2) and Fe. These equations of states are multi-phases, include liquid and solid phases, and aim at building planetary and exoplanetary interior models solely based on ab initio predictions. This talk will concentrate on the results obtained for MgSiO3 and its dissociation products MgO and SiO2 where we used ab initio predictions, laser shock experiments combined with XANES (X-ray near edge spectroscopy) measurements to study the physical properties of these constituents at planetary core conditions.

This work is supported in part by the French Agence National de la Recherche under contract PLANETLAB ANR-12-BS04-0015.

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High pressure phase diagram of MgO and FeO

D. Cebulla, R. Redmer

University of Rostock

The state of matter (e.g. temperatures and pressures) inside super-Earths, i.e., planets in the mass range 1-10 ME, is much more extreme than in the interior of the Earth so that current experiments are not able to cover the whole density-temperature range directly [1]. In order to improve the understanding of the interior of exoplanets and their physical properties [2], ab inito calculations for the planetary materials are needed.

Typical representatives are MgO and FeO, which are abundant materials in the Earth's mantle. Both are expected to be also important for the mantle of exoplanets as well as for the rocky cores of gas giants such as Jupiter [3]. Using ab initio molecular dynamic simulations (VASP [4]), we have determined the phase diagram for MgO up to 20000 K and 1.5 TPa. In particular, the transition from the solid to the molten salt has been studied using diffusion analyses and pair distribution functions. The transition from the NaCl (B1) to the CsCl (B2) structure in solid MgO is determined by calculating the respective free enthalpies. The phase diagram of MgO is constructed based on the accurate equation of state (EOS) data. We compare with experimental results from (decaying) shock and ramp compression experiments [5, 6]. The B1-B2 and the liquid-solid transition line are compared with earlier simulation and experimental results [7].

The more complex phase diagram of FeO is under investigation, first results with DFT+U calculations show agreement with experimental results for the B1 phase. Using the quasi-harmonic approximation the EOS is calculated and compared against available experimental data [8].

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Decaying shock studies of the MgO and $MgSiO_3$ high pressure phase diagrams and implications for Earth-like and super-Earth planets

R. Bolis[1], G. Morard[2], T. Vinci[1], A. Ravasio[1], E. Bambrink[1], M. Guarguaglini[1], M. Koenig[1]; R. Musella[3], F. Remu[3], J. Bouchet[4], N. Ozaki[5]; K. Miyanish[5], T. Sekine[6], Y. Sakawa[7], T. Sano[7], R. Kodama[5], F. Guyot[2], A. Benuzzi-Mounaix[1]

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MgO and $MgSiO_3$ are among the most abundant components of Earth-like and Super-Earth planets. A detailed knowledge of phase diagrams, melting curves and liquid properties is of fundamental importance for modelling the internal dynamics of these rocky exoplanets. E.g. planetary temperature profiles are controlled by the melting of mantle components [1].

Here we report an experimental investigation of the Hugoniot high pressure-temperature (P-T) states of MgO and $MgSiO_3$ performed with laser-driven decaying shocks at the LULI and GEKKO facilities. We focused 1.2-2.5 ns laser pulses with an intensity between 3-8 1013 W/cm2 reaching P-T states along the Hugoniot between 150 GPa and 1 TPa and 6000 K and 30000 K. We determine the P-T states using rear side optical diagnostics. For MgO, we observed a single transition associated to melting (at 0.47 TPa ± 0.04 and 9863 ± 812 K), while for $MgSiO_3$ we had no evidence of any transition in the range 150-500 GPa.

Some implications are presented comparing our data with experimental and theoretical data found in literature [2, 3, 4, 5, 6, 7]. In particular our observations do not confirm the occurrence of a liquid-liquid transition in $MgSiO_3$, topic that constitutes an unsolved controversy [3, 6] and that has important geophysical implications related to geochemical differentiation in exoplanets. Moreover, we propose a revision of the phase diagram of MgO, with a lower melting line which results in a lower temperature profile for super-Earths. Furthermore, for both materials, we observed that metallization and melting do not occur at coincident thermodynamic conditions (reflectivity starts to increase at P-T along the Hugoniot higher than melting), implying the presence of poorly electrically conducting liquid. This result constitutes an important input for modelling the magnetic field generation via dynamo mechanism. In summary, we propose a new interpretation of MgO and $MgSiO_3$ phase diagrams at high P-T conditions to be accounted for when modelling super-Earths.

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A computational framework of mantle thermodynamics

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Determining phase equilibria and physical properties of mineral phases is a critical tool in the characterization of the state of the mantle in the Earth and other terrestrial planets and hinges both on the availability of experimental data and physically meaningful descriptions of the data within a thermodynamic model. Such models are required to advance different fields in solid Earth geophysics such as geodynamics and seismology.

The experimental database is at a point where the thermodynamic description can be made in a meaningful way. We have developed an efficient, object-oriented, extensible software framework to facilitate such computations that can accommodate different models for the equation-of-state and thermal parts, and hence use various databases that are appropriate for different geological questions. A stable phase assemblage is computed by minimizing Gibbs energy for a given composition and a set of mineral phases, allowing for solid solutions with different endmembers. The program also computes physical properties as derivatives of Gibbs energy. Here we present and discuss results on the thermal and elastic structure for the Earth's mantle.

Session 5: Phase transitions

Structural transitions in shock-compressed hydrocarbons

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Hydrocarbons at pressures of few Mbar and temperatures of several thousand Kelvins are present in icy giant planets and in the first compression phase of ablator materials in contemporary inertial confinement fusion concepts. Here we show structural transitions at 0.5-2 Mbar pressure achieved by shock compression and double-shock compression of polystyrene and polyethylene probed with in situ X-ray diffraction and spectrally resolved X-ray scattering at LCLS. For strong shock compression we observe a fluid with strong short-time bonding of the carbon atoms, possibly leading to de-mixing. For double-shocked polystyrene, we record de-mixing and phase separation into diamond and hydrogen, as suggested to happen inside Neptune and Uranus, on nanosecond timescale.

Ultra-high pressure equation of state using laser compression

A. Lazicki[1], F. Coppari[1], R. J. Rygg[1], R. Smith[1], D. Fratanduono[1], R. Kraus[1], J. McNaney[1], G. Collins[1], D. Swift[1], R. London[1], D. Erskine[1], H. Whitley[1], J. Castor[1], J. Nilsen[1], J. Eggert[1], D. McGonegle[2], J. Wark[2]

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The evolution of crystal structure in compressed solids, and the Hugoniot equation of state together form a critical basis for formulation of broad-ranging equation of state models, used to describe and predict properties of matter at extremes of temperature and pressure in the interiors of giant planets and stars. Using laser compression, it is now possible to experimentally achieve material states at pressures far beyond the upper limit of data commonly found in the literature; in some cases into regimes where new genres of physical properties have been predicted but so far unverified. We will present measurements of crystal structure in solid carbon to the 20 Mbar pressure regime using in-situ x-ray diffraction, with direct relevance for understanding properties of carbon-rich astronomical bodies. We will also discuss plans and preliminary results for an effort to extend the Hugoniot equation of state of metals to pressures of hundreds of Mbar.

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Warm Dense Carbon on XFELs

Dr. N. Hartley

Helmholtz Zentrum Dresden Rossendorf

Carbon is one of the most abundant elements in the universe, and is a major constituent of Uranus and Neptune, as well as believed to be an present in many newly-discovered exoplanets. However, the properties of carbon at high pressure and temperature conditions are still poorly understood, with XFELs offering a unique way to study the behaviour with unprecedented detail. This talk will look at recent results from the LCLS and SACLA facilities, as well as discussing future experiments.

The phase diagram of water under extreme conditions of pressure and temperature

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At extreme pressures of several megabars and temperatures of several thousand Kelvin, dissociation and ionization of water molecules leads to a transition from the molecular liquid to a dense nonideal plasma. In the low-temperature solid, the molecular ice VII transforms into the ionic ice X, which is accompanied by dynamical disordering in the proton dynamics and symmetrization of hydrogen bonds. State-of the- art computer simulations predict that a large area of the phase diagram is covered by exotic superionic phases, that are embedded between the dense ices and the nonideal plasma. Superionic water is characterized by highly mobile protons that diffuse through a crystalline oxygen lattice [1,2].

Here we use ab initio computer simulations to investigate the thermodynamic and transport properties of water under extreme conditions. The method is a combination of classical molecular dynamics (MD) simulations for the ions and density functional theory (DFT), which allows for a quantum description of interacting electrons. We calculate basic thermodynamic quantities like pressure, internal energy, and entropy in order to parametrize analytic thermodynamic potentials for ices VII and X [3] and for superionic water [4]. Phase boundaries between the dense ices and two superionic phases (with bcc and fcc oxygen lattice) are calculated as well. We also discuss how the type of the oxygen lattice in the superionic phase influences transport properties like the electrical conductivity. Our results are of significant importance not only for a fundamental understanding of the behavior of water under extreme conditions, but also for application in the interior modeling of water-rich giant planets like Uranus and Neptune.

Session 6: Diagnostics of shocked metals

Structure factor measurements in strongly coupled plasmas in the long wavelength limit

P. Neumayer

GSI Helmholtz Zentrum für Schwerionenforschung

We present measurements of the static structure factor in high energy density matter. Angle-resolved x-ray scattering was performed at the Matter at Extreme Conditions (MEC) instrument at the Linac Coherent Light Source (LCLS). Strongly coupled warm-dense aluminium was produced by laser shock compression using the MEC high-energy long pulse laser system. Scattering of 8 keV probe radiation from the FEL was spectrally resolved by highly efficient scattering spectrometers to distinguish quasi-elastic and inelastic scattering components. Covering a wide range of scattering angles with unprecedented angular resolution the correlation peak of the ion-ion structure factor could be well resolved, providing direct determination of the ion-ion distance and thus the ion density. The exceptional collimation of the LCLS beam enabled measurements at small scattering angles, thus accessing small scattering k-vectors while using x-rays sufficiently hard to penetrate the dense plasma. Our measurements provide stringent benchmark to structure factor calculations which are strongly model dependent at these large scale lengths. We have realized k-vectors down to 0.3/A, approaching the long wavelength limit, where the material compressibility is fundamentally linked to the ion-ion structure factor via the compressibility sum rule. This holds the potential for a novel approach to measure compressibility of HED matter.

Doing time-resolved synchrotron x-ray measurements at very high pressure: a strategy and first results.

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Over the past 20 years, putting diamond anvils cells in front of synchrotron beamlines has permitted tremendous progress in the high pressure field. However, this static high pressure approach is now facing its limits, and won't go much higher in extreme P-T conditions due to the diamond non-infinite mechanical constants.
Now, doing time-resolved measurements seems to be the way to progress in the study of the very dense matter. To date, time resolved x-ray diffraction in the one-second range has permitted to overcome the chemical contamination problems arising during the determination of melting curves by laser-heating inside a DAC[1]. We will present here our recent developments of two dynamical high P-high T generation devices acting in two different time ranges : 1) the Ramp heating DAC (µs) and 2) the laser shock compression setup (ns). We have started to couple these devices with the ESRF XAS and XRD beamlines. Our first results will illustrate the possibilities of these techniques: a micro-second time resolved X-ray absorption approach to measure the XANES spectra of Fea in the Warm Dense Matter regime[2] and a nano-second time resolved measurement, by doing laser shock compression to produce EXAFS measurements of Fe and Ta much outside the static domain ([3] and Figure 1).

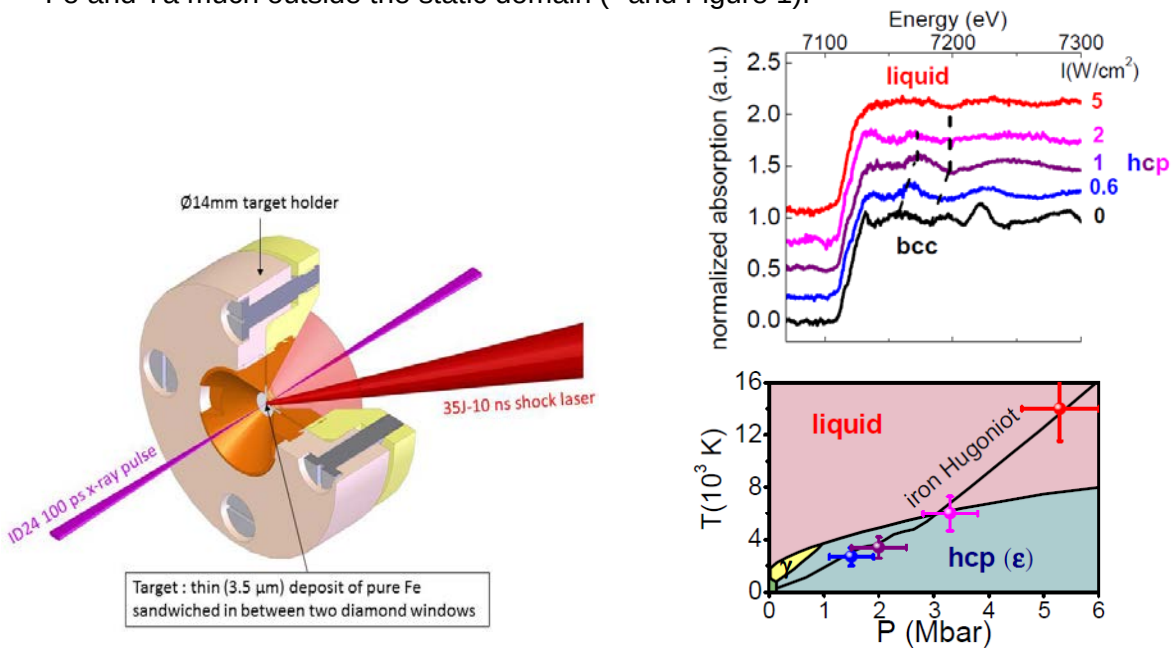

Figure 1: left panel; Schematic view of the shock laser (red) hitting the target while the ESRF-ID24 single pulse (purple) probes the warm dense state of matter. Right panel; TOP: EXAFS spectra from the target acquired with laser power up to 510^{13} W/cm^2 allowing to follow a trend to the liquid phase. BOTTOM: iron phase diagram showing the corresponding P-T points (same colors).

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Ab initio simulations of the dynamic ion structure factor of warm dense lithium

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We perform molecular dynamics simulations based on finite-temperature density functional theory in order to determine self-consistently the static and dynamic ion structure factor and the electronic form factor in lithium. This comprehensive data set allows for the extraction of the dispersion relation for collective excitations, the calculation of the sound velocity, and the determination of the ion feature that is given by the total electronic form factor and the static ion structure factor. The results are compared with available experimental x-ray and neutron scattering data. A very good agreement is obtained for both the liquid metal and warm dense matter domain. Finally, we study the impact of possible inhomogeneities in the target on the x-ray scattering spectrum.

Session 7: Metals at HP-HT

Complex Structures in Shock-Compressed Scandium to 82 GPa.

McMahon

The University of Edinburgh

Under static compression, Sc transforms to an incommensurate host-guest (H-G) composite structure at 21 GPa at 300 K. While such complex structures have also been found in other elements in DAC experiments, it is not known whether they can form on the sub-nanosecond timescales of a shock compression experiment. in collaboration with colleagues from Oxford, Euro-XFEL, AWE, LLNL, LANL and LCLS, have recently shocked Sc to 82 GPa on the MEC beamline at the LCLS, and observe three phases transitions on compression: hcp to bcc at ~33 GPa, bcc to the H-G phase at 46 GPa, and then melting between 53 and 72 GPa. The quality of the diffraction data is such that we can determine that the chains of guest atoms in the H-G phase are disordered above 2000K - as seen previously in K and Rb. These results are consistent with recent results from a high-P high-T DAC study, and can be combined into a single phase diagram.

Time resolved x-ray diffraction: dynamics of pressure induced structural phase transition in bismuth

Z. Jenei

Lawrence Livermore National Laboratory

High brightness synchrotrons and fast high performance detectors allow direct measurement of the characteristics of structural phase transitions at rapid compression rates. We have used the dynamic diamond anvil cell at 3rd generation synchrotron facilities to study pressure induced phase transitions at slow (2-3 GPa/s) to fast (1 TPa/s) compression rates. The compression rate can dramatically influence the microstructure of metals and the location of the phase boundaries in pressure-temperature space. We explore the rich phase diagram of bismuth and discuss the effects of compression rate on solid-to-solid phase transition pressures. We will also show measurements of the solid-liquid phase transitions in gallium.

This work performed under the auspices of the US DOE by LLNL under Contract DEAC52-07NA27344.

Time-resolved XANES spectroscopy using a table-top laser-plasma source: study of copper under extreme conditions and out-of-equilibrium

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Ultrashort laser sources development enables nowadays the possibility for matter to reach both solid density and high temperature (~10 000 K) conditions, or what we call « Warm Dense Matter ». Neither plasma physics nor condensed matter models are able to give a good description of how matter behaves during this intermediate state. Lots of experimental and theoretical works are now in progress in this research field. Moreover, working with femtosecond lasers leads to out-of-equilibrium phenomena during which a large mount of energy is deposited in the electrons while the lattice remains cold. Resulting thermal equilibration and phase transitions dynamics are still on the debate. A lattice is predicted by quantum molecular dynamics simulations applied to noble metals (gold, silver, copper). This would be due to the stability reinforcement of the crystalline lattice, also known as “bond hardening” [1]. The latter is linked to the electronic d-band shift towards low energies, and has been invoked to interpret an electron diffraction experiment on a gold sample [2]. There is still a need for experimental evidence of this phenomenon.

XANES spectroscopy would be a way to experimentally highlight it. A study of the copper near the L3-edge (932 eV) using a synchrotron source has been recently published [3]. Electronic d-states are probed from 2p3/2-states. A pre-edge is observed to be building up, which evolution gives the electronic temperature dynamics.

The shift of the electronic d-band during the out-of-equilibrium conditions may generate a spectral shift of this pre-edge, but hasn’t been evidenced yet. We also think that the loss of the crystalline order should give rise to the disappearance of the post-edge structures.

Several experiments have been realized using Eclipse laser and a table-top station dedicated to time-resolved XANES measurements at CELIA laboratory [4]. At first, XANES spectra have been acquired using an x-ray source produced by the irradiation of a CsI solid target. This source duration of ~15 ps FWHM (approximately the equilibration thermal time of copper) restrained our temporal resolution. We used more recently a xenon clusters jet to produce an x-ray source of comparable emissivity but a significantly shorter duration of ~2.5 ps FWHM. Out-of-equilibrium XANES spectra have been measured and show the same pre-edge evolution as the one published by LNBL. Signal over noise ratio allows us to follow the evolution of the post-edge structure and deduce the associated dynamics of the loss of crystalline structure.

The observation of a spectral shift of the pre-edge and the validation (or not) of the « bond-hardening » requires an even shorter temporal resolution. This should be soon achieved by the mean of a betatron x-ray source at LOA.

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Non-Drude conductivities in isochorically heated warm dense aluminum observed by inelastic x-ray scattering

P. Sperling[1], B. Witte[2], L. Fletcher[2], E. Galtier[2], E. Gamboa[2], H. J. Lee[2], U. Zastrau[1,2], R. Redmer[3], S. Glenzer[1]

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[3]University of Rostock

We have performed highly-resolved inelastic x-ray scattering measurements in warm dense aluminum isochorically heated by 8 keV Linac Coherent Light Source (LCLS) photons. The inelastic forward scattering spectra resolve electronic density fluctuations (plasmons) that allow an accurate determination of the electron density, electron temperature, and for the first time the electrical conductivity [1]. The latter is infered from the plasmon peak position and width that is strongly affected by electron-particle interactions causing plasmon damping smaller than calculated by Landau damping.

We present density functional theory molecular dynamic (DFT-MD) simulations of the electrical conductivity of warm dense aluminum that show non-Drude conductivities indicating electron-particle collisions as well as electron excitation. Translated into a plasmon spectrum we find a very good agreement with our measurements previously not achieved by standard perturbative theories due to an insufficient description of dissipative processes in strongly coupled plasmas.

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Electronic transport properties of metals at extreme conditions

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Electrical resistivity ρ_{el} and thermal conductivity $\lambda_{th}$of metals at high density and temperature are crucial parameters for the evolution of planetary dynamos. Although the widely-used Kubo-Greenwood formalism can provide good results for both quantities, it is computationally expensive and restricted to small simulation cells of a few hundred atoms on contemporary machines. As an alternative approach for calculating electrical resistivity of metals, Ziman-type formulae

$$\rho_{el} = \frac{a_0\hbar}{e^2}\frac{4\pi^3 Z}{a_0 k_F}\frac{1}{(2k_F)^4}\int_0^{2k_F} S(q)\,|u(q)|^2 q^3 dq$$

have been used for both liquids and warm solids. Here, $\frac{a_0\hbar}{e^2} \approx 21.74\ \mu\Omega$cm is the atomic unit of resistivity, Z the number of valence electrons, k_F the Fermi wavenumber and $q = |k - k'|$ the scattering wavenumber. This formulation is easily generalizable to multi-component systems and can be used to estimate λ_{th} with the law of Wiedemann-Franz.

The spatial arrangement of scattering centers, which is described by the static ion-ion structure factor $S(q)$, can be obtained from a computationally cheap force-field molecular dynamics simulation with good accuracy and for large cells. Problems occur upon mapping the quantum-mechanical nature of electron-ion interaction onto a screened pseudo-potential $u(q)$. Resistivity values from semi-empirical model potentials of a Heine-Abarenkov type are very sensitive to parameters due to the strong q^3 weight and fail at quantitatively reproducing experiments, particularly for *d*-electron metals. Attempts of replacing $u(q)$ by the transition matrix elements of a specifically constructed muffin-tin potential have been more successful in this respect, yet somewhat cumbersome in implementation. We currently investigate possible improvements to semi-empirical model potentials of the Heine-Abarenkov-type in order to reproduce experimental resistivity values for alkalines and Kubo-Greenwood values for liquid aluminum.

Posters

From Giant Planets to Fusion Energy

M. Aykul

Boğaziçi University

As we known that WDM is located at the cores of giant planets such as Jupiter and Saturn. However, it can be found in high temperature and high pressure. Producing power from WDM requires different kinds of accelerators. In this poster, I would like to introduce the facilities which try to reveal fusion energy from warm dense matter, and their techniques and components. The Neutralized Drift Compression Experiment II can be the example for this goal.

Equations of state for molecular mixtures in the interior of Uranus

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[4]University of California, Santa Cruz

The interior of the giant planet Uranus is dominated by a mixture of the molecular compounds water, ammonia and methane. Many observable properties of this planet, such as luminosity, gravitational moments and magnetic field, are thought to be determined by the physical and chemical properties of matter within this ice layer. Hence, the phase diagrams, equations of state and structural properties of these materials and their respective mixtures are of great interest. [1]

Here, we investigate binary 1:1 mixtures as well as the 4:1:2 water-ammonia-methane mixture performing density functional theory molecular dynamics simulations using the VASP code. [2] In particular, the widely used linear mixing approximation for equations of state is verified for the conditions present inside Uranus' interior ranging up to 10 Mbar. [3] Additionally, the diffusive properties are calculated for the ternary mixture along the planetary profile.

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Numerical models for magnetic field generation in the ice giants

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The magnetic fields of the ice giant planets Uranus and Neptune are multipolar and non- axisymmetric. Voyager-II-data and HST aurorae-observations suggest magnetic power spectra with similar power in the first three spherical harmonic degrees and a peak in the order m=1. Multipolar, non-axisymmetric fields can be modeled with many approaches including a high density stratification in the dynamo region, strongly turbulent convection, a dynamo generated by fast zonal jets and a geometrical setup with a deep stably stratified fluid layer below the dynamo region. Earlier studies of the latter found multipolar fields and in a few cases reproduced the peak in the magnetic power spectra at order m=1 (Stanley and Bloxham, 2006). Here we explore the robustness of the link between the multipolarity (similar power for l=1,2,3) and the m=1-peak and a deep stably stratified layer below the dynamo region using 3D numerical dynamo models. We compare our results to internal structure models of the ice giants in order to constrain the parameters and geometrical setups that are in accordance with the magnetic field observations.

Development of the EXAFS diagnostic onthe National Ignition Facility

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[2]LLE

The use of lasers to induce extreme compression states has enabled the study of material properties and equations of state at unprecedented pressures and temperature conditions [1].

The combination of laser-driven compression and x-ray diagnostics provides a unique picture of the transformations taking place in high energy density matter in nanosecond time scales.

In static high pressure experiments, X-ray diffraction (XRD) and x-ray absorption spectroscopy (XAS) are the principal diagnostics used to characterize structural properties and document the occurrence of phase transitions. Recently we have developed these capabilities at the Omega laser (University of Rochester, NY) to look at phase transitions of matter dynamically driven to high pressure and high temperature [2, 3, 4, 5]. Here we present the first attempt at developing XAS measurements at the National Ignition Facility (NIF) (Lawrence Livermore National Laboratory, CA) where much higher compression can be achieved.

We use 128 laser beams and about 400kJ to implode a 1.5mm diameter plastic capsule acting as x-ray source. As the capsule implodes it becomes hot and eventually generates a bright, smooth and broad-band x-ray flash (bang time). A flat crystal spectrometer is used to disperse the x-rays generated by the implosion in the 7 keV range and an image plate detector is used to record EXAFS spectra at the Fe K-edge [5].

Different capsule sizes and materials have been studied to optimize the x-ray source. Their brightness is compared and discussed together with the achieved spectral resolution.

These measurements represent the first attempt at measuring EXAFS spectra on the NIF. Future experiments will allow us to extend the measurements to laser-driven samples and to look at different materials, by changing the dispersive crystal in the spectrometer.

Performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344.

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Interior structure models for exoplanets of different composition and their Love number k_2 values

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Institute of Physics, University of Rostock

The increasing number of discovered exoplanets provides us with new planetary classes, such as super-Earths and mini-Neptunes. In order to model their interior structure the mean density of a planet is an important input. Based on this quantity we can decide whether extensive gaseous layers or rocky mantle materials have to be considered.

In this work we calculate three-layer models with an adiabatic outer layer of volatile material and isothermal, solid inner mantle (MgO) and core (Fe) as well as the resulting Love numbers k_2. This quantity results from the planet's internal density profile and, if also measured, can be used to constrain the possible layer compositions and sizes.

To examine the effect of planet mass, layer sizes and surface temperature on internal structure and Love number we perform a parameter study. Furthermore, we apply the results to analyze several known exoplanets with measured densities in the regime of super-Earths and mini-Neptunes. We find that an observational constraint on k_2 would be particularly useful to narrow down the planetary Fe/MgO mass ratio.

Fabrication of Al-Ce Impendence Matching Target and EOS Study of Cerium

C. Lu, D. Ren, H. Zhang, D. Zhang, P. Shi

Institute of Materials, China Academy Of Engineering Physics

Shock wave compressing experiment is a major way to obtain equation of state (EOS) data for materials at ultra-high dynamic pressure and temperature. In ambient environment, cerium (Ce) is easily oxidized and distorted because of its high activity. So it is very inconvenient to fabricate EOS targets of Ce by traditional method, especially micro-scale EOS targets. Therefore, we apply focused ion beam (FIB) technology to the fabrication of micro-scale Al-Ce impendance matching target. The targets fabricated by FIB has little oxidization, high accuracy, and high rate of products. By shock wave compression experiment, EOS data of Ce at near TPa pressure is achieved for the first time and is in good accordance with previous EOS of Ce. The compression ratio is as high as 3.55. The EOS data is helpful to study the phase transition properties of Ce at ultra-high dynamic pressure.

X-ray diffraction form uniaxially compressed fiber textured polycrystalline

D. McGonegle

University of Oxford

When materials are compressed beyond their Hugoniot elastic limit, they act to relieve built up shear stress by deforming plastically. Tantalum provides an interesting case to study owing to its multitude of competing plasticity mechanisms, a combination of dislocation and deformation twinning. We perform in situ X-ray diffraction in order to investigate deformation mechanisms of shock compressed fibre textured tantalum over a range of shock pressures up to 270 GPa along (110) direction. Previous studies have shown twinning occurs at lower pressures. Here, we present the first direct, in situ observation of twinning in shock compressed metals, and demonstrate that twin fraction increases with shock pressure reaching a twin dominated plastic response at 40-50 GPa. We find that above 150 GPa the dominant plastic mechanism is slip. These results are compared to molecular dynamics simulations performed using the Ravelo potential, showing the onset of twinning at a similar pressure.

Toward high-accuracy modeling of Jupiter's gravity field

N. Nettelmann, R. Redmer

University of Rostock

This summer, the Juno spacecraft has entered into orbit around Jupiter. Juno is a solar-powered NASA mission with the scientific goal of providing insight to the structure and evolution of the giant planet Jupiter through improved understanding of its atmospheric winds, interior dynamics and dynamo generated in the metallic H-He envelope, and to the internal density distribution. The latter is susceptible to both the size of a rocky core -a fundamental prediction from planet formation theory- and to the equation of state of high-pressure H-He mixtures. To achieve these goals, Juno carries instruments to measure the atmospheric O/H ratio down to ~ 100 bars, the geometry of the magnetic field, and the gravity field to high accuracy of 1:10^9.

Analysis of the expected high-accuracy gravity data requires the development of new theoretical methods and numerical modules. This presentation is concerned with recent progress in that regard by other authors [1-4], and with the own attempt to catch up with those.

The observable gravity field can (but perhaps should not [3]) be separated into the influence from a rigidly rotating body, which emerges most strongly at low orders (2k<8) in the spherical harmonic decomposition, and from deep or atmospheric differential rotation, which appear as high-order (2k>6) gravity field perturbations. To compute the gravity field to high accuracy, Hubbard (2012, 2013) has developed the theory of Concentric Maclaurin Spheroids. Here, we will present the current status of implementing this method. Our effort will serve to predict the gravity field of a rigidly rotating Jupiter based on the most recent Rostock H-He EOS [5]. Subtraction of this contribution from the observed gravity data will then allow to access the properties of Jupiter's atmospheric and internal dynamics.

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Dispersion Forces and Metallization in Dense Liquid Helium

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Helium as the second most abundant element in the universe is of great importance for the modeling of giant gas planets such as Jupiter and Saturn. For instance, an accurate equation of state (EOS) is needed for their interior and evolution models. Density Functional Theory (DFT) combined with classical Molecular Dynamics (MD) is an efficient and robust method to calculate the EOS of matter under extreme conditions as they are relevant for planetary interiors.

In this context, the inclusion of dispersion forces in DFT will potentially allow us to describe warm dense matter, especially noble gases, more accurately. On this poster the influence of different functionals for dispersion forces on the EOS of helium is examined for a wide range of densities and temperatures.

Recently, strong evidence for a nonmetal-to-metal transition in dense liquid hydrogen was found [M. Knudson et al., Science 348, 1455 (2015)]. We perform EOS and conductivity calculations in order to identify the temperature and pressure conditions under which helium shows a similar electronic transition. If the transition is of first order, jumps in certain thermodynamic functions should occur. However, no discontinuities were found. Furthermore, the results for the conductivity show no evidence for a first order phase transition, either.

Calculations of phonons spectra from ab-initio MD simulation

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As major components of Earth and probably of most of small and mid-sized exoplanets, MgO and Iron at high conditions of pressure and temperature require a particular interest in the scope of planetary model ling. We used a method recently proposed by O. Helman et al. [PRB84180301(2011)] to determine the vibrational properties of a system and taking into account temperature effects via ab-initio molecular dynamics. In particular, we examine the elastic properties of MgO and the compressional sound velocity of iron.

The new method (Temperature Dependent Effective Potential method) developed at CEA allowed us to go beyond the thermal dilatation (QuasiHarmonicApproximation). Thanks to this method, we show the domain of validity of this approximation in the case of MgO. We also calculate the elastic constants of MgO. Going deeper inside planetary interior, the sound velocity of iron needs accurate studies to understand its dependence on alloys density and to quantify anharmonic effects at high temperature. Ohtani et al. (2015) and Antonangelli et al. (2012) seem to show a linear dependence of the sound velocity VP of pure iron with respect to density up to1000K (Birch law). But Mao et al. (2012), with the same technic, conclude to power-law evolution of VP. We have used the same method TDEP, as done for MgO, in ab initio molecular dynamics simulations to determine sound velocities and elastic constants of pure iron in its hexagonal closed-packed phase.

Mercury's core evolution

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Remote sensing data of Mercury's surface by MESSENGER indicate that Mercury formed under reducing conditions. As a consequence, silicon is likely the main light element in the core together with a possible small fraction of sulfur. Compared to sulfur, which does almost not partition into solid iron at Mercury's core conditions and strongly decreases the melting temperature, silicon partitions almost equally well between solid and liquid iron and is not very effective at reducing the melting temperature of iron. Silicon as the major light element constituent instead of sulfur therefore implies a significantly higher core liquidus temperature and a decrease in the vigor of compositional convection generated by the release of light elements upon inner core formation.

Due to the immiscibility in liquid Fe-Si-S at low pressure (below 15 GPa), the core might also not be homogeneous and consist of an inner S-poor Fe-Si core below a thinner Si-poor Fe-S layer. Here, we study the consequences of a silicon-rich core and the effect of the blanketing Fe-S layer on the thermal evolution of Mercury's core and on the generation of a magnetic field.

Adiabatic connection fluctuation-dissipation (ACFD) theory-based equation-of-state of hcp iron

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The large discrepancy in equation-of-state estimates for hcp iron between experiments and computations based on density functional theory (DFT) have been a source of concern for more than 20 years, putting the question of magnetism in hcp Fe at the center of attention. While computations within DFT using generalized gradient approximations (GGA) to exchange and correlation (xc) find a stable magnetic structure at P<50 GPa, there is – at best – ambiguous indication of magnetism from experiments.

Typical functionals of representing xc are based on (semi-)local approximations and lead to systematic errors, such as the self-interaction error or the inaccurate description of the negative ions, with the potential not showing an asymptotic 1/r Coulomb decay. The adiabatic connection fluctuation-dissipation (ACFD) theory provides – in principle – an exact evaluation of xc energy within DFT. Within ACFD the Hartree xc energy E_Hxc is separated into E_H, and an exact evaluation of E_x, based on the KS wavefunctions, plus the ACFD formulation of E_c. For evaluation of E_c the random phase approximation is used that ignores xc kernel in evaluating the ACFD integral. Here we perform calculations on the equation-of-state of nonmagnetic hcp iron to test whether within the ACFD theory the description of hcp Fe improves when compared to experiments and whether the magnetic structure described previously may be artificially stabilized by DFT-GGA.

We find that the equilibrium volume of hcp Fe from the ACFD computations is expanded significantly when compared to non-spin-polarized results using GGA, at the same level as magnetism does within DFT-GGA. However, the compressibility does not decrease appreciably to bring DFT-based computations in closer agreement with experiments.

Atmosphere–interior co-evolution: Implications for the long-term evolution of the global carbon cycle

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The global carbon cycle plays a key role in regulating the Earth's climate by controlling the concentration of CO_2 in the atmosphere. Its long-term stability is provided by internally-driven processes such as the presence of plate tectonics [1]. However, the tectonic regime of planetary bodies may depend on surface temperature according to recent geophysical studies of Venus [2, 3]. To study the complex interplay between interior dynamics and climate evolution, we present a geophysical model that simulates the cycling of carbon through all relevant reservoirs. A special emphasis is placed on the effect of different convective regimes on both degassing and regassing efficiency. By systematically varying the critical yield stress, our numerical calculations suggest that planets with mobile plates on top of the convecting mantle outgas significantly more CO_2, when compared to their one-plate counterparts. For mobile-lid convection, degassing rates are mainly driven by volcanic activities at regions where cold surface material is transported into the interior. Elevated volcanic activity ensures a steady CO_2 flux from the interior to the atmosphere, which is, in the long run, balanced by removal of atmospheric CO_2 due to silicate weathering. For stagnant-lid convection, degassing is controlled by hot upwellings originating at the core-mantle boundary. Since these mantle plumes need time to rise to the surface, we observe extended periods in which no CO_2 is released into the atmosphere, leading to strong fluctuations in atmospheric CO_2 concentration and surface temperature.

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Calibrating mixing-length theory for highly viscous fluids

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The internal dynamics and thermal evolution of terrestrial planets is mainly governed by the efficiency of convective heat transfer through the viscous mantle [1]. Since it is computationally challenging to investigate a large parameter space while precisely modelling the full convective heat flux, parameterized descriptions of thermal convection are essential. A simple method to calculate quickly the convective heat transport is known as the mixing-length theory [2, 3]. In this study, we present a calibration of the mixing-length parameter in the local mixing-length theory. The parameterization is derived from a comparison between sophisticated three-dimensional (3-D) numerical experiments and the one-dimensional (1-D) mixing-length theory with a varying mixing length. We find that the mixing length depends on both viscosity contrast and Rayleigh number of the convective system. Moreover, different convective regimes could be identified and corresponding scaling relationships for the mixing length are presented. For mobile-lid convection at low to medium viscosity contrasts, mixing length has to be larger when compared to its conventional formulation as distance to the nearest thermal boundary. Furthermore, peak depth of the mixing length occurs in the mid- region of the convective system. For stagnant-lid convection at high viscosity contrasts, mixing length is substantially lower and its peak depth is found at greater depths. The proposed calibration establishes the mixing-length theory as simple 1-D approach for calculating the thermal evolution of rocky planets.

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