Matter under Extreme Conditions

732. WE-Heraeus-Seminar

20 Oct - 23 Oct 2020
at the Physikzentrum Bad Honnef/Germany

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HERAEUS-STIFTUNG

Subject to alterations!

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 732. WE-Heraeus-Seminar:

With the detection of the first extrasolar planet in orbit around a main sequence star in 1995 began a new era of planetary and astrophysics. To this day, almost 4000 exoplanets have been detected, and of approximately 700 we know both the radius and mass and therefore an average density which permits a classification. Among the various different types of exoplanets discovered, (i) super-Earths and (ii) mini-Neptunes have generated a specific interest in planetology. These classes represent planets with (i) an average density similar to that of the terrestrial planets in our solar system and a mass of up to 10 ME, and (ii) the density of the ice giants with a mass of a few ME, respectively. At the center of a super-Earth with 5 ME, pressure reaches values of 2 TPa and temperatures are expected in the range of 8,000 K. In order to characterize the internal structure of exoplanets and to decrease uncertainty on their composition, knowledge of physical properties of planetary matter at these conditions is required:

- Thermodynamic properties provide information on the internal structure of the planet via equations-of-state, and density distribution within the planet in turn permits the prediction of observables such as moment of inertia or the fluid Love number.
- Electric and thermal conductivity determine whether a planet may operate a dynamo and thereby generate a magnetic field. The (indirect) observation of magnetic fields of exoplanets has just begun in astronomy.

Advances in high pressure generation using both static and dynamic techniques as well as the in-situ characterization of samples give access to the relevant conditions for the first time, provide parameters for planetary modelling, and permit a cross-check for material properties computed using ab-initio methods.

Scientific Organizers:

Prof. Dr. Ronald Redmer — Universität Rostock, Germany
E-mail: ronald.redmer@uni-rostock.de

Dr. Gerd Steinle-Neumann — Bayerisches Geoinstitut, Universität Bayreuth
E-mail: g.steinle-neumann@uni-bayreuth.de

Dr. Zuzana Konôpková — European XFEL GmbH, Germany
E-mail: zuzana.konopkova@xfel.eu

Program

Program

Tuesday, 20 October 2020

17:00 – 21:00	Registration	
from 18:30	*BUFFET SUPPER / Informal get together*	

Wednesday, 21 October 2020

07:30 – 08:30	*BREAKFAST*	
08:30 – 08:45	Gerd Steinle-Neumann	**Welcome**

Session 1: Experiments (Chair: Carmen Sanchez Valle)

08:45 – 09:25	Leonid Dubrovinsky (online)	**Structureal studies above 100 Gpa: surprises and challenges**
09:25 – 10:05	Hauke Marquardt (online)	**Experiments on planetary materials in dynamically-driven diamond anvil cells**
10:05 – 10:30	*COFFEE BREAK*	
10:30 – 11:30	Stewart McWilliams (online)	**Beeing there : What to do with TeraPascal pressure experiments**
11:30 – 11:50	Sergey Lobanov (online)	**Time-resolved measurements of optical properties at extreme P-T conditions**
11:50 – 12:10	Johannes Kaa (online)	**High pressure and temperature X-ray emission and diffraction studies of iron containing minerals at the European XFEL**
12:10 – 12:30	**Discussion**	
12:30 – 12:40	**Conference Photo** (in front of the Lecture Hall)	
12:40	*LUNCH*	

Program

Wednesday, 21 October 2020

Session 2 : Ionized Matter (Chair: Thomas Tschentscher)

14:00 – 15:00	Dominik Kraus (on site)	**Studying Ionization in Dense Plasmas**
15:00 – 15:40	Ulf Zastrau (online)	**Time-resolved XUV and X-ray methods at high-intensity laser facilities**
15:40 – 16:10	Oliver Humphries (online)	**Mapping the Electronic Structure of Warm Dense Nickel via Resonant Inelastic X-ray Scattering**
16:00 – 16:30	*COFFEE BREAK*	
16:30 – 17:10	June Wicks (online)	**Shock experiments on and off the Hugoniot**
17:10 – 17:50	Nick Hartley (online)	**High-pressure hydrocarbon chemistry relevant to planetary interiors**
17:50 – 18:10	Trevor Hutchinson (online)	**How dense z-pinch velocimetry can constrain models of warm dense aluminum**
18:10 – 18:30	**Discussion**	
18:30	*HERAEUS DINNER at the Physikzentrum (cold & warm buffet, with complimentary drinks)*	

Program

Thursday, 22 October 2020

07:30 – 08:30	*BREAKFAST*	
Poster Session: (Chair: Ronald Redmer)		
08:30	Poster flash	
10:00 – 10:30	*COFFEE BREAK*	
10:30	Poster flash continued	
12:30	*LUNCH*	
14:00 – 15:30	**Poster Session**	
Session 3: Exoplanets: (Chair: Gerd Steinle-Neumann)		
15:30 – 16:30	Ansgar Reiners (online)	**A guided tour through observations of planets outside the solar system**
16:30 – 17:00	*COFFEE BREAK*	
17:00 – 17:40	Szilard Csizmadia (online)	**Constraining the interiors of exoplanets by measuring the Love number k_{2f}**
17:40 – 18:20	Nadine Nettelmann (online)	**Constraining the interior of fluid planets by using Love number measurements**
18:20 – 19:00	Sabrina Schwinger (online)	**Interior evolution models as link between planetary composition and structure**
19:00 – 19:20	Philipp Baumeister (online)	**Shaping the atmospheres of terrestrial planets with interior-atmosphere feedback processes**
19:30	*DINNER*	

Program

Friday, 23 October 2020

07:30 – 08:30	*BREAKFAST*	
Session 4: Ab-initio (Chair: Ronald Redmer)		
08:30 – 09:30	Taku Tsuchiya (online)	**Physical properties of Minerals in the Ultrahigh—ressure Planetary Interior Conditions from Ab Initio Computations**
09:30 – 10:10	Martin French (online)	**Ab initio simulations for physical properties of molecular HCNO mixtures**
10:10 – 10:40	*COFFEE BREAK*	
10:40 – 11:20	Gerd Steinle-Neumann (on site)	**Phase transitions in silicates at the conditions of super-Earth interiors**
11:20 – 11:40	Liang Yuan (on site)	**Hydrogen in the Earth's core**
11:40 – 12:10	**Discussion**	
12:10 – 12:30	Ronald Redmer	**Closing remarks**
12:30	*LUNCH*	

End of the seminar and *FAREWELL COFFEE* / **Departure**

Posters

Posters

01	Alexis Amouretti (online)	**Hematite phase diagram under laser shock compression**
02	Donato Belmonte (online)	**Melting phase relations at extreme conditions: a thermodynamic approach based on phase diagrams calculation**
03	Armin Bergermann	**Gibbs-Ensemble Monte-Carlo simulations for binary mixtures**
04	Mandy Bethkenhagen (online)	**Carbon ionization at gigabar pressures: An *ab initio* perspective on astrophysical high-density plasmas**
05	Katerina Falk (online)	**The use of structured targets to enhance x-ray line emission for probing of warm dense matter**
06	Timofey Fedotenko	**Synthesis and compressibility of novel nickel carbide at pressures of Earth outer core**
07	Sandeep Kumar	**Ionization and transport in the multi-component plasma of Hot Jupiter atmospheres**
08	Dominic Langhammer	**A two component model for silicate melt viscosity**
09	Hanns-Peter Liermann (online)	**Progress in using XFELs to unravel the superionic character of ice in planetary environments**
10	Julian Lütgert	**Structural properties of shock-compressed polyethylene terephthalate**
11	Xiayun Pan (online)	**Investigation of hot dense plasmas heated by short-pulse intense laser using x-ray spectroscopy**

Posters

12	Christian Plueckthun	**Investigating the effect of compression rates on the stress development in experiments using the dynamic diamond anvil cell (dDAC) technique**
13	Esther Posner (online)	**Atomic-scale insight into the material properties of liquid iron alloys as a function of pressure, temperature, and composition**
14	Martin Preising	**Metallization of dense fluid helium from ab initio simulations**
15	Ludwig Scheibe	**Influence of a thermal boundary layer on the thermal evolution of Uranus and Neptune**
16	Maximilian Schörner	***Ab initio* analysis of x-ray Thomson scattering**
17	Jie Yao	**$MgSiO_3$-SiO_2 eutectic at lower mantle pressure from multi-anvil experiments**

Abstracts of Lectures

(in chronological order)

Structureal studies above 100 GPa: surprises and challenges

Leonid Dubrovinsky
[1]BGI, University of Bayreuth, Bayreuth, Germany
Leonid.Dubrovinsky@uni-bayreuth.de

The impact of high-pressure studies on fundamental physics and chemistry, and especially on the Earth and planetary sciences, has been enormous. Modern science and technology rely on the fundamental knowledge of matter that is provided by crystallographic studies. The most reliable information about crystal structures and their response to changes in pressure and temperature is obtained from single-crystal diffraction experiments. Advances in diamond anvil cell (DAC) techniques and double-stage DACs, as well as in modern X-ray facilities have increased the accessible pressure range for structural research up to multimegabar range. We have developed a methodology to perform single-crystal X-ray diffraction experiments in double-side laser-heated DACs. Our results demonstrated that the solution of crystal structures, their refinement, and accurate determination of thermal equations of state of elemental materials, oxides, carbides, borides, carbonates, and silicates from single-crystal diffraction data are possible well above 100 GPa at temperatures of thousands of degrees. These resulted in findings of novel compounds with unusual compositions, crystal chemistry, and physical properties. We illustrate application of new methodology for simultaneous high-pressure and high-temperature single crystal diffraction studies using examples of investigations of chemical and phase relations in the Fe-O system, transition metals carbonates, silicates, nitrides, and hydrides.

Experiments on planetary materials in dynamically-driven diamond anvil cells

H. Marquardt[1], Alba San José Mendéz[2,3], Rachel Husband[3], and Hanns-Peter Liermann[3]

[1]Department of Earth Sciences, University of Oxford, Oxford, United Kingdom
[2]Bayerisches Geoinstitut, University of Bayreuth, Germany
[3]Deutsches Elektronen Synchrotron DESY, Germany

Dynamic diamond-anvil cells (dDACs), where sample compression is achieved by a piezoeletric actuator, facilitates compression of planetary materials at variable compression rates and along customised compression paths. The combination with time-resolved synchrotron x-ray diffraction allows for tracking the material's response to compression with a practically continuous pressure-resolution, even at high temperatures [1]. Here, I will present some of our recent high-pressure dDAC results on planetary materials, including H_2O ice VII/X and (Mg,Fe)O. I will show how the novel experimental data reveal subtle changes of the compression behavior induced by phase transitions. I will discuss approaches to constrain the materials' elastic bulk modulus at high pressure directly from the experimental data without assuming a specific equation of state formalism.

References

[1] A.S.J Mendez et al., Review of Scientific Instruments **91**, 073906 (2020).

Being there: What to do with TeraPascal pressure experiments

R. Stewart McWilliams[1]

[1]*School of Physics and Astronomy and Centre for Science at Extreme Conditions, University of Edinburgh, Peter Guthrie Tait Road, Edinburgh EH9 3FD, UK*

With increasing and diverse ways to reach very high pressures in the laboratory – from those occurring within planets such as Earth, to those found within massive planets and even stars – we need sophisticated methods to excite, transform, and study the extreme states of matter produced. Ultra-high pressure measurements place demands on speed, sensitivity, and scale that are being met in the current generation of novel experimental techniques. In this talk I will review the types of probes and excitations uniquely suited for work at these very high pressures, using modern ultrabrilliant light sources such as free electron lasers and ultrafast measurements in table top to stadium sized laboratories. This talk will cover how traditional measurements are constantly being enhanced, combined, diversified, and regenerated with the help of new technologies and the growing communities and bigger collaborations working at extreme pressures.

Time-resolved measurements of optical properties at extreme P-T conditions

S. S. Lobanov[1], Lukas Schifferle[1], Reiner Schulz[1]

[1]GFZ German Research Centre for Geosciences, Section 3.6, Telegrafenberg, 14473 Potsdam, Germany

Optical studies of materials at high pressure-temperature (P-T) conditions provide insights into their physical properties that may be inaccessible to direct determination at extreme conditions. Incandescent light sources, however, are insufficiently bright to optically probe samples with radiative temperatures above ~1000 K. At the meeting, we will report on a new experimental setup at GFZ that allows optical experiments in a laser-heated diamond anvil cell at T up to at least 4000 K [1]. This setup is based on a pulsed supercontinuum (broadband) light probe and a gated CCD detector. Precise and tight synchronization of the detector gates (3 ns) to the bright probe pulses (1 ns) diminishes the recorded thermal background and preserves an excellent probe signal at high temperature. Using this new instrumentation we were able to measure optical absorbance of solid and molten $(Mg,Fe)SiO_3$, an important constituent of planetary mantles, at P ~30 GPa and T ~1200-4150 K (Figure 1). Our setup enables quantitative estimates of the opacity of planetary mantles with implications to their thermal and electrical conductivity, all of which have never been constrained at representative P-T conditions.

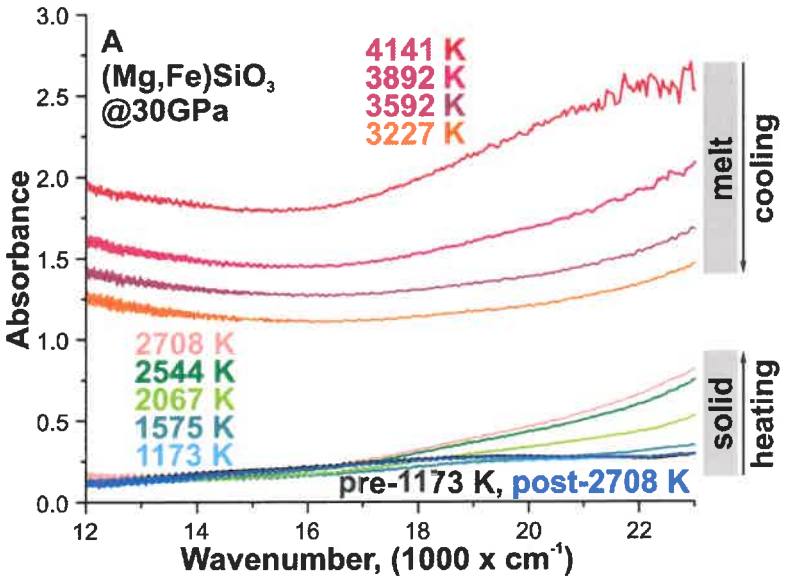

Figure 1. High temperature optical absorption spectra of $(Mg,Fe)SiO_3$ at 30 GPa (~18 μm thick). The arrows schematically depict that optical measurements in the solid/molten sample were performed upon a gradual increase/decrease of the laser heating power.

References

[1] S. S. Lobanov et al., Review of Scientific Instruments, 91, 053103 (2020)

High pressure and temperature X-ray emission and diffraction studies of iron containing minerals at the European XFEL

J. Kaa[1,2], C. Albers[2], K. Appel[1], V. Cerantola[1], M. Elbers[2], L. Libon[3], M. Makita[1], A. Pelka[1], S. Petitgirard[4], C. Plueckthun[1], T. R. Preston[1], C. Sahle[5], R. Sakrowski[2], A. Schmidt[1], G. Spiekermann[4], C. Sternemann[2], M. Tolan[2], M. Wilke[3], U. Zastrau[1], Z. Konopkova[1]

[1]European XFEL GmbH, Schenefeld, Germany, [2]TU Dortmund, Dortmund, Germany, [3]University of Potsdam, Potsdam, Germany, [4]ETH Zürich, Zürich, Switzerland, [5]European Synchrotron Radiation Facility ESRF, Grenoble, France

The understanding of the spin state of iron is crucial for our understanding of chemical and physical properties of the deep Earth's interior. Nevertheless, data on the spin state of iron bearing minerals and iron alloys that compose Earth's interior are scarce at high temperatures and pressures, due to limitations of the commonly used techniques to heat and probe the spin state *in-situ*, especially at core-mantle-boundary conditions and beyond.

To overcome these limitations, we conducted an experiment with a different approach by measuring simultaneous X-ray emission (XES) and X-ray diffraction (XRD) on Siderite ($FeCO_3$) pressurized to 52 GPa within a diamond anvil cell (DAC), at the High Energy Density instrument (HED) at the European XFEL [1]. We used the unique properties of a pulsed and highly brilliant X-ray free electron laser (XFEL) beam that allowed us to heat samples contained in a DAC via isochoric X-ray heating, a method that was developed by the efforts of the EuXFEL Community Proposal #2292. This way we were able to heat and probe the sample with the same X-ray pulse train utilizing a pink beam with an energy of 13 keV. We collected the Fe Kβ fluorescence, which is sensitive to the spin state [2], using a van Hamos spectrometer with a single Si (5,3,1) analyzer crystal and simultaneously measured the XRD to directly probe the samples structural changes including a spin change induced volume change [3].

Using both *in-situ* and *ex-situ* measurements, we identified the decomposition phases Magnetite-h (Fe_3O_4), tetracarbonates ($Fe_4C_3O_{12}$), CO_2 and melt, suggesting heating of the sample above 3000 K while using a pulse energy of 250 µJ during the experiment. This successful proof of principle of combining XES, XRD in a DAC using an XFEL beam opens up unique possibilities to probe the spin state of pressurized samples at very high temperatures in solid and molten systems relevant for deep planetary interiors.

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[3] Liu, J., Lin, J., Prakapenka, V. High-Pressure Orthorhombic Ferromagnesite as a Potential Deep-Mantle Carbon Carrier. Sci Rep 5, 7640 (2015). https://doi.org/10.1038/srep07640

Studying Ionization in Dense Plasmas

D. Kraus[1,2]

[1] *University of Rostock, Rostock, Germany*
[2] *Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany*

Ionization is a key property of every plasma. At high densities and moderate temperatures, comparable to the interiors of giant planets and small stars, bound states can be significantly affected by the surrounding medium. Moreover, free electrons are partially degenerate which additionally complicates the prediction of ionization balances and related properties. Today, state-of-the-art facilities like X-ray Free Electron Lasers or the National Ignition Facility open unique possibilities to study this regime of matter to provide valuable constraints for stellar and planetary models. I will review several recent experiments and discuss some ongoing developments.

Time-resolved XUV and X-ray methods at high-intensity laser facilities

U. Zastrau[1] et al.

[1]High Energy Density Science, European XFEL, Schenefeld, Germany

In my talk, I will give a selected examples of methods using X-ray ultra violet (~90 eV or 13.5 nm), soft (~1..2 keV) and hard x-rays to diagnose matter in extreme conditions. These will conclude pumping (also called heating) with these x-rays and creating extreme states, as well as probing extreme states which have been created by other means.

Due to the lack of time, the talk cannot give a complete overview, but I will concentrate on results that have been achieved at free-electron laser facilities. I will touch the first results that have been obtained at the first SASE FEL "FLASH" as early as 2008-2014, namely creating transparent aluminium, L-shell conution band spectroscopy and heating of hydrogen. Then I will present the first results from the LCLS from 2010 on soft x-ray pumped plasmas, which yield insight into ionization potential lowering and opacity. Finally, at the end I will pick a few inelastic x-ray scattering examples to show the possibility of diagnosing the electronic system and the dielectric funtctions via plasmons, and the ionic motion via phonon spectroscopy.

References

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Mapping the Electronic Structure of Warm Dense Nickel via Resonant Inelastic X-ray Scattering

O. S. Humphries[1]*, R. S. Marjoribanks[2], Q. van den Berg[3], E. C. Galtier[4], M. F. Kasim[3], H. J. Lee[4], A. J. F. Miscampbell[3], B. Nagler[4], R. Royle[3], J. S. Wark[3] and S. M. Vinko[3]

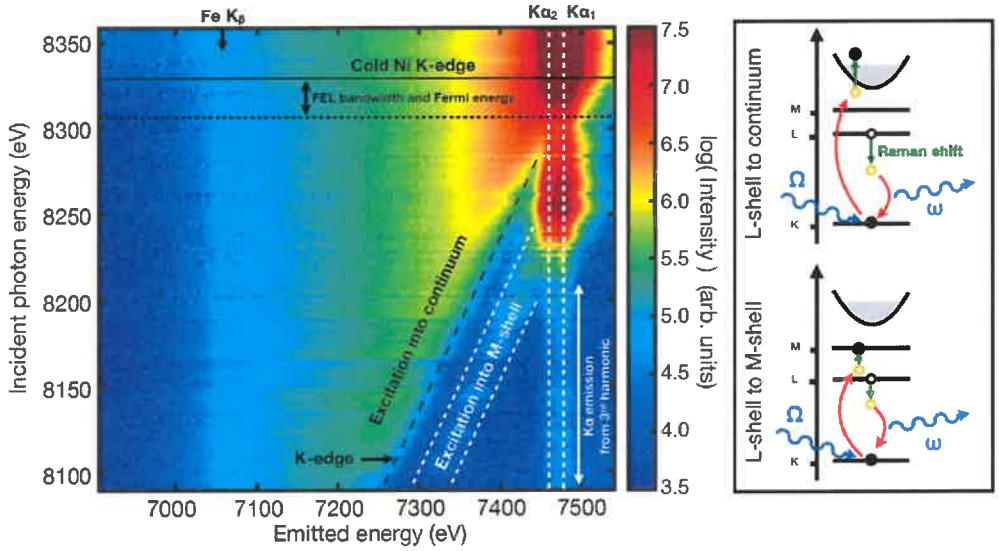
[1] *Department of Radiation Physics, Bautzner Landstraße 400, 01328 Dresden, Germany*

[2] *Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario, M5S 1A7, Canada*

[3] *Department of Physics, Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX1 3PU, UK*

[4] *Linac Coherent Light Source, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA*

**o.humphries@hzdr.de*



The development of bright free-electron lasers (FEL) has revolutionised our ability to create and study materials in the warm-dense matter and high-energy-density (HED) regimes. Current diagnostic techniques have been successful in yielding information on fundamental thermodynamic plasma properties, but provide only limited or indirect information on the detailed quantum structure of these systems, and on how it is affected by ionization dynamics. Here we show how the electronic structure of solid density nickel, heated to temperatures of 10's of eV on femtosecond timescales, can be studied by resonant inelastic x-ray scattering (RIXS) using the Linac Coherent Light Source FEL. We present single-shot measurements of the valence structure of the x-ray-heated transient system, and simultaneously extract electron temperatures, ionization, and ionization potential energies. The RIXS spectrum provides a wealth of information on the HED system that goes beyond what can be extracted from x-ray absorption or emission spectroscopy alone.

Shock experiments on and off the Hugoniot

J. Wicks[1], Zixuan Ye[1], Raymond Smith[2], and Marius Millot[2]

[1] Earth & Planetary Sciences, Johns Hopkins University, Baltimore, USA
[2] Lawrence Livermore National Laboratory, Livermore, CA, USA

High pressure and temperature conditions of minerals found in large Super-Earth interiors are experimentally accessible using dynamic compression using either laser or pulsed-power drivers [1]. Paired with in situ diagnostics such as x-ray diffraction and optical pyrometry, shock and ramp compression experiments probe the high pressure and temperature phase diagram. However, differences in measurement diagnostic type and potential kinetic effects potentially obscure the true, equilibrium phase boundary, resulting in discrepancies between experimental studies and theoretical calculations.

In this lecture, I will describe various laser-driven dynamic compression experiments on MgO that interrogate the phase boundary conditions, the transition mechanism, and optical depth across the B1-B2 phase boundary. We compare these experiments to recent measurements [2,3] and calculations [4,5] of the phase transitions of MgO along the shock Hugoniot, and consider discrepancies between studies in the context of experimental timescales. We will discuss the upcoming opportunities and challenges of laser-driven dynamic compression studies on high pressure mineralogy.

References

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High-pressure hydrocarbon chemistry relevant to planetary interiors

N. J. Hartley

SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

The mantles of icy giant planets such as Uranus and Neptune are dominated by light elements. Understanding the chemistry that is induced by the pressures and temperatures present is therefore essential to understanding such bodies [1]. This has the potential to explain the complex magnetic field structures and the differences in observed heat flux, but also has implications for exoplanets throughout the galaxy, where ice-dominated planets appear common.

In order to better understand the chemical and structural behavior occurring inside these planets, we have carried out a series of experiments, at facilities around the world, using plastic samples and laser shock compression to recreate planetary mantle conditions in the laboratory. These compressed samples have been studied with diffraction, showing diamond formation [2]; inelastic scattering, which probes species separation [3]; and optical diagnostics, to study thermal behavior [4], among others.

While these results are exciting in their own right, they also demonstrate the current state of dynamic compression experimental facilities, particularly in combination with X-ray diagnostics. These approaches will be essential as we move towards liquid samples which more closely recreate the expected mantle composition [5], leading to further insights into planetary behavior and evolution.

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How Dense Z-pinch Velocimetry Can Constrain Models of Warm Dense Aluminum

T.M. Hutchinson[1], T.J. Awe[2], B.S. Bauer[1], D.H. Dolan[2], J.R. Pillars[2], B.T. Hutsel[2], E.P. Yu[2], A.W. Klemmer[1], and S.E. Kreher[1]

[1]University of Nevada, Reno, Nevada 89506, USA

[2]Sandia National Laboratories, Albuquerque, New Mexico 87185, USA

Photonic Doppler Velocimetry (PDV) was recently used [1] to measure the exploding surface of metal driven by lineal electric current density increasing at 3 x 10^15 A/m/s. Aluminum-6061 rods are driven to 850 kA in approximately 100 ns, with the metal thicker than the skin depth. According to PDV, the metal surface melts at 85 T and expands with a constant acceleration. Then, at surface magnetic field 140-180 T, the metal acceleration begins to increase in time. These data have proven to be sensitive discriminators for EOS tables in magnetohydrodynamic modeling of warm dense matter. We will present the data, new analysis, and briefly cover preliminary 1D MHD modeling.

References

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Constraining the interiors of exoplanets by measuring the Love number k_{2f}

Sz. Csizmadia, H. Hellard

[1]*Deutsches Zentrum für Luft- und Raumfahrt, Institut für Planetenforschung, Berlin, Germany*

The two most important planet parameters, the mass and radius – and thus the density derived from them – select the possible theoretical planetary interior models. Usually, they are many and the models are degenerated: more than one possible composition, interior structure, density profile match the observed planetary mass and radius and these models differ from each other significantly.

To narrow the ranges of the possible interior models, we clearly need at least one more observable. Among others, we also proposed that certain Love-numbers can play the role of a third measured parameter [1,2,3]. These Love-numbers are direct functions of the internal density profile of a celestial body. When they are measured, then they can be used for further and significant downselection of the models [4].

In this talk we present how these Love-numbers can be determined form transit photometry, transit timing variations and radial velocity observations of exoplanets. After the theory we investigate the feasibility and disturbing factors and how to manage them. We also present the first results of the feasibilty studies and first estimates [5,6,7] and we report new, recently obtained measurements which are based on our recent HARPS-runs.

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Constraining the interior of fluid planets by using Love number measurements

N. Nettelmann[1]

[1]*Institute of Planetary Research, DLR Berlin, Germany*

This talk focuses on results from internal structure and evolution modeling of fluid planets. Fluid planets including Jupiter and Neptune are at the center of understanding high-density matter, planet formation, and the workings of planetary systems. Fluid planets are fluid because they are warm (several 1000 K-100,000 K) and consist mostly of H and He, making them unique astrophysical laboratories to test H-He equations of state and phase diagrams. In addition, we are interested it the mass fraction and radial distribution of ices (C/N/O), refractory elements (Si,Fe,Mg), and inert elements (He,Ne,Ar,Kr,Xe). Of the solar system giants we know that the heavy elements are not homogeneously distributed. How do we know? Fortunately, gravity is a long-range force that is not impeded in an opaque, hostile environment such as planetary interiors are. Love numbers k_{nm} are linear response coefficients of the planetary gravity field subject to tidal perturbation. The era where k_{22} of fluid exoplanets can be measured has begun [1].

In this talk I will summarize our understanding of the solar system giants based on gravity measurements and discuss how k_{22} can be used to infer internal composition distribution of exoplanets. We distinguish between tidal/fluid and static/dynamic Love numbers. Jupiter's k_{22} value observed by Juno has just slipped away from the predicted static value [2]; pioneering measurements for fluid exoplanets may also suggest strong dynamical effects at play. Thus, Love number k_{22} computations offer new challenges and opportunities in planetary science.

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Interior evolution models as link between planetary composition and structure

S. Schwinger[1]

[1]*German Aerospace Center (DLR), Rutherfordstr. 2, 12489 Berlin, Germany*

Large scale melting by giant collisions is an inevitable consequence of terrestrial planet formation by planetesimal accretion. Hence not only terrestrial planets in our solar system but also the majority of terrestrial exoplanets might have experienced a magma ocean (MO) phase characterized by global and maybe even complete melting of their silicate fraction.

The process of MO solidification is linked to the differentiation of the planetary interior into different chemical reservoirs, that can be modified by convection and partial melting processes throughout the history of the planet. Such interior differentiation processes can be modeled to assess a) which chemical reservoirs form and b) how they are distributed in the interior at the present day. The physical properties and radial positions of individual reservoirs are directly linked to potentially observable physical properties of the bulk planet like its density or moment of inertia. Therefore, interior evolution models that simulate magma ocean solidification, solid state convection and ideally decompression melting can act as a link that connects bulk planetary composition and structure.

We have applied such a modeling approach to the evolution of the Moon in order to constrain the bulk silicate Moon (BSM) FeO content, which is difficult to establish based solely on petrological arguments. We first used petrological modeling to study the effect of BSM FeO content on the properties of chemical reservoirs in the lunar mantle that were formed during lunar magma ocean solidification. In a second modeling step, we considered the effects of solid state convection on the distribution of these reservoirs in the lunar interior. The results are used to test the consistency of different BSM FeO contents and mantle convection scenarios with the bulk Moon density and BSM moment of inertia. Combining current estimates of the lunar core properties and today's selenotherm with our lunar interior models, we find that BSM FeO contents of 8 – 13.5 wt% are consistent with the observed bulk Moon properties. Further constraints on the lunar interior structure from seismic and selenodetic data (suggesting e.g. the presence of a dense, partially molten zone at the core mantle boundary [1]) indicate that BSM FeO contents of 9 – 11 wt% are most probable. This estimate could be further limited by tighter constraints on the size and density of the lunar core, e.g. by future seismic investigations.

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Shaping atmospheres of terrestrial planets with interior-atmosphere feedback processes

P. Baumeister[1], N. Tosi[2], J. MacKenzie[1], J. Grenfell[2], M. Godolt[1]

[1]Zentrum für Astronomie und Astrophysik, Technische Universität Berlin, Berlin, Germany

[2] Deutsches Zentrum für Luft- und Raumfahrt (DLR), Berlin, Germany

During the lifetime of a terrestrial planet, the evolution of its atmosphere is mainly driven by volcanic outgassing of volatiles from the planet's interior [1]. Outgassing rates are shaped by feedback processes in both the interior and the atmosphere, which are influenced by several factors, such as the initial mantle volatile content affecting convection in the mantle as well as the possibility to produce partial melts, and atmospheric pressure limiting the outgassing of volatiles from surface melts [2]. We use a 1D parameterized convection model to simulate the evolution of H_2O and CO_2 outgassing into the atmospheres of terrestrial exoplanets, including feedback processes between interior and atmosphere, and utilize a chemical equilibrium model to describe the composition of the atmosphere over time. We are conducting an extensive parameter study to investigate a wide range of initial conditions, including, among others, the initial water content of the mantle, its redox state, the initial surface pressure of a primordial atmosphere, the planet's mass, and the ratio between planetary core and mantle size. For planets with cores smaller than Earth's, the atmosphere tends to be dominated by CO_2, whereas H_2O is the main atmosphere component for planets with larger cores. Furthermore, the total mass of the atmosphere remains largely constant throughout the evolution of the planet, regardless of the initial surface pressure.

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Physical properties of Minerals in the Ultrahigh-Pressure Planetary Interior Conditions from Ab Initio Computations

T. Tsuchiya[1], H. Dekura[1], and S. Ritterbex[1]

[1]Ehime University, Matsuyama, Japan

Pressure and temperature conditions of the interiors of super-Earths and giant planets are extremely high. Since experimental measurements of physical properties of materials in such conditions are quite difficult or nearly impossible due to technical difficulty, non-empirical theoretical calculation is an important alternative approach. In particular, ab initio density functional simulation is a quite powerful technique due to its high predictability and wide applicability. This technique can be applied to investigate several properties of silicate and oxide minerals, including not only fundamental equilibrium properties (e.g., P,V,T equations of state and high-P,T phase relations [1,2]) but also more complicated transport and rheological properties (e.g., thermal conductivity [3,4,5] and viscosity [6,7]), which help to model the planetary interior dynamics more quantitatively.

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Ab initio simulations for physical properties of molecular HCNO mixtures

M. French[1]

[1]*Institute of Physics, Rostock, Germany*

Mixtures of the molecular compounds water, ammonia, and methane (HCNO mixtures) are the main constituents of the so-called Ice Giants Uranus, Neptune, as well as exoplanets of similar category [1]. At the extreme planetary interior conditions, these molecular substances become dissociated and ionized. They may also transform into superionic compounds or even partially demix from each other.

In this talk, I will present results from ab initio computer simulations based on density functional theory that yield predictions for the phase diagram and the equation of state of HCNO compounds. Understanding planetary HCNO mixtures in their full complexity requires especially profound knowledge of the behaviour of the individual components. In this regard, ab initio calculations allow us to systematically examine how well mixing rules for the equation of state can offer opportunities for a simplified understanding [2].

In addition to thermodynamic properties, transport properties like the electrical and thermal conductivity are highly important for modelling the magnetic field generation and thermal evolution processes in giant planets. This talk will report on recent progress achieved in calculating conductivity, viscosity, and Prandt number of water at planetary interior conditions [3]. Especially, the influence of dissociation and ionization on the electrical and thermal conductivity will be discussed.

The results presented here can be directly applied in the development of novel planetary structure and evolution models for the Ice Giants that allow us to gain a better understanding of their nature.

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Phase transitions in silicates at the conditions of super-Earth interiors

G. Steinle-Neumann[1], Florian Trybel[1] and Dominic Langhammer[1]

[1] *Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany*

An improved description of the internal structure of extrasolar super-Earths requires a detailed understanding of phase relations and material properties at pressures (P) and temperatures (T) up to 1 TPa and 10,000 K. As for the terrestrial planets in our solar system, the mantles of super-Earths must be dominated by compositions in the SiO_2-MgO system, with varying Mg/Si ratios characteristic for their host starts [1]. In the Earth's lowermost mantle, mineralogy is dominated by the $MgSiO_3$ post-perovskite phase and MgO. At P beyond those in the Earth's interior, MgO has been shown experimentally [e.g., 2,3] and computationally [e.g., 4,5] to undergo a phase transition from the B1 to the B2 structure, although no agreement has been reached on the exact transition P and the Clapeyron slope. Transitions in the full MgO-SiO_2 system, by contrast, have only been characterized by computations, based on structure predictions [e.g., 6-8]. These simulations have reached a general consensus on the silicate compositions and structures, involving unexpected MgO/SiO_2-ratios, e.g., $MgSi_2O_5$ [7]. However, as for the MgO B1-B2 transition, the location of equilibrium between different phase assemblages remain poorly constrained. This is partly due to the different methods applied that may, for example, not be able to sufficiently characterize structures outside their P-T stability range. Here we review different computational approaches and results for phase equilibria by looking at the MgO B1-B2 and the $MgSiO_3$ perovskite to post-perovskite transitions.

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Hydrogen in the Earth's core

Liang Yuan and Gerd Steinle-Neumann

Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany

The Earth's core is the main repository for many of the planet's elements and determining its composition is a major goal in understanding the state and evolution of Earth's interior. A large number of elements have been proposed to account for the density deficit of the core, i.e., its lower density compared to pure iron. Among them is hydrogen, the most abundant element in the universe whose budget on Earth is uncertain as it is volatile and escapes Earth's gravitational field readily.

Despite its importance, the amount of hydrogen in the core has been poorly understood as it is extremely difficult to measure the hydrogen content in iron metal from experiments at high pressure and temperature. Here we explore the distribution of hydrogen between silicate and iron liquid, corresponding to equilibration during core formation in the magma ocean of the young Earth. We use density-functional-theory based molecular dynamics to perform coexistence simulations and thermodynamic integration which provide qualitative and quantitative information on element partitioning, respectively.

Abstracts of Posters

(in alphabetical order)

Hematite phase diagram under laser shock compression

A. Amouretti[1], M. Harmand[1], A. Boury[1], F. Guyot[1], D. Kraus[2], O. Mathon[3], S. Pascarelli[3], C. Pepin[4], K. Rohatsch[2], A. Schuster[2], N. Sévelin-Radiguet[3], A. Sollier[4], R. Torchio[3], M. Zhang[2], G. Fiquet[1], A.Benuzzi-Mounaix[5], T. Vinci[5], B. Albertazzi[5], M. Koenig[5], A. D. Chin[6]

[1]Institut de Minéralogie de Physique des Matériaux et de Cosmochimie, CNRS, Sorbonne Université, MNHN, Paris, FRANCE
[2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, GERMANY
[3]ESRF, Grenoble, FRANCE
[4]CEA-DAM-DIF, Arpajon, FRANCE
[5]LULI, École Polytechnique, CNRS, CEA, UPMC, Palaiseau, FRANCE
[6]Laboratory for Laser Energetics, University of Rochester, Rochester, UNITED STATES

Until recently, iron oxides were assumed to comprise only FeO, Fe_3O_4, and Fe_2O_3. However, static compression experiments have demonstrated the existence of new iron oxide stoichiometries at high pressure and temperature such as FeO_2 [1], Fe_4O_5 [2], Fe_5O_6 [3]. These discoveries, with the wide variety of iron oxides phases existing at high pressure [4], highlight the complexity of iron-oxygen phase diagram at extreme condition. In this context, measurements of physical properties, phase transition processes and phase diagrams of Fe-O systems with laser shock compression techniques offer opportunities to extend the actual pressure and temperature ranges of such studies. Here, we will present main results from a laser shock experiment at the ID24 ESRF beamline using time-resoved X-ray absorption measurement on Fe_2O_3 samples. In addition, we will show result from a recent experiment performed at LULI 2000 to measure equation of state and calculate sound velocities along the Fe_2O_3 Hugoniot and above 500GPa.

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Melting phase relations at extreme conditions: a thermodynamic approach based on phase diagrams calculation

D. Belmonte[1]

[1]*DISTAV, University of Genoa, Genova, Italy*

Despite the outstanding progress in computer technology and experimental facilities, understanding melting phase relations in planetary interiors is still an open challenge. In this work a computational scheme to predict melting phase relations at HP-HT by a combination of first principles DFT calculations, polymer chemistry and equilibrium thermodynamics is presented and discussed. The adopted theoretical framework is physically-consistent and allows to compute multi-component phase diagrams in a broad range of P-T conditions by a simplex convex-hull algorithm for Gibbs free energy minimization [1]. The calculated phase diagrams are in turn used to simulate the P-T-X evolution of magmas in planetary interiors, providing some thermodynamic constraints on both present-day and early Earth melting processes. High-pressure melting curves of mantle silicates, as well as original insights on the evolution of liquid-liquid miscibility gaps under pressure, are also obtained as by-product of phase diagram calculation [2]. Application of the above method to the CaO-MgO-Al_2O_3-SiO_2 (CMAS) system and relative subsystems highlights as pressure effects are not only able to change the nature of melting of some minerals (like olivine and pyroxene) from eutectic to peritectic (and vice versa), but also simplify melting relations by drastically reducing the number of phases with a primary phase field at HP-HT conditions.

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Gibbs-Ensemble Monte-Carlo simulations for binary mixtures

A. Bergermann, M. French, M. Schöttler and R. Redmer

Institut für Physik, Universität Rostock, D-18051 Rostock, Germany

We explore the performance of the Gibbs-Ensemble Monte-Carlo simulation technique by calculating the miscibility gap of H_2-He mixtures with analytical exponential-six potentials [1]. We calculate several demixing curves at pressures up to *500* kbar and at temperatures up to *1800* K. Our results are in good agreement with *ab initio* simulations in the non-dissociated region of the phase diagram. Next, we determine new parameters for the Stockmayer potential [3] to model the interactions in the H_2-H_2O system at temperatures of *1000* K < *T* < *2000* K. The corresponding miscibility gap of H_2-H_20 mixtures was explored by using the same Gibbs-Ensemble Monte-Carlo simulation technique. We calculated demixing curves at pressures up to *150* kbar and at temperatures up to *2000* K. Our results show reasonable agreement with previous experimental data of Bali *et al* [2].

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Carbon ionization at gigabar pressures: An *ab initio* perspective on astrophysical high-density plasmas

Mandy Bethkenhagen[1,2], Bastian B. L. Witte[1,3], Maximilian Schörner[1,3], Gerd Röpke[1], Tilo Döppner[4], Dominik Kraus[5,6], Siegfried H. Glenzer[3], Philip A. Sterne[4], Ronald Redmer[1]

[1]*University of Rostock, Institute of Physics, 18051 Rostock, GERMANY*
[2]*CNRS, École Normale Supérieure de Lyon, Laboratoire de Géologie de Lyon, 69364 Lyon, FRANCE*
[3]*SLAC National Accelerator Laboratory, Menlo Park, CA 94025 USA*
[4]*Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*
[5]*Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, GERMANY*
[6]*Institute of Solid State and Materials Physics, Technische Universität Dresden, 01069 Dresden, GERMANY*

A realistic description of partially ionized matter in extreme thermodynamic states is critical to model the interior and evolution of the multiplicity of high-density astrophysical objects. Current predictions of its essential property, the ionization degree, rely widely on analytical approximations that have been challenged recently by a series of experiments [1-2]. Here, we propose an ab initio approach to calculate the ionization degree directly from the dynamic electrical conductivity using the Thomas-Reiche-Kuhn sum rule [3]. This density functional theory framework captures genuinely the condensed-matter nature and quantum effects typical for strongly correlated plasmas. We demonstrate this capability for carbon and hydrocarbon, which most notably serve as ablator materials in inertial confinement fusion experiments aiming at recreating stellar conditions. We find a significantly higher carbon ionization degree than predicted by commonly used models, yet validating the qualitative behavior of the average atom model PURGATORIO. Additionally, we find the carbon ionization state to remain unchanged in the environment of fully ionized hydrogen. Our results will not only serve as benchmark for traditional models, but more importantly provide an experimentally accessible quantity in the form of the electrical conductivity.

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The use of structured targets to enhance x-ray line emission for probing of warm dense matter

Katerina Falk

Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics,
Dresden, Germany

Determining the plasma conditions of Warm Dense Matter (WDM) is very challenging due to near solid densities and relatively low temperatures (0.1 - 100 eV). Thus, active x-ray probing is crucial to determine the equation of state and transport properties of such plasmas at conditions relevant to the planetary interiors. Ultrashort high intensity laser pulse irradiation of solid targets generates very high temperature, high density plasma emitting bright x-ray emission with short pulse duration and high peak brightness that can use used for a variety of applications including x-ray radiography, x-ray Thomson scattering and/or isochoric heating of targets to the WDM regime. For these applications very bright-x-ray sources are required. Introducing structures in the solid targets with size in the order of the laser wavelength can significantly enhance the energy conversion from laser to target is expected to be improved greatly [1]. Such structures can increase the laser absorption fraction and/or increase the density and temperature of the generated hot electrons further facilitating the generation of X-ray emission from the target. Some past experiments have demonstrated enhancement both of He-alpha lines as well as K-alpha lines depending on the target and laser parameters [2,3]. In this work we present novel experiments with nano-structured Cu wire targets carried out at the Trident laser at the Los Alamos National Laboratory. Spectroscopic measurements have observed enhancement of He-alpha emission and evidence of increased plasma temperature and improved ionisation fraction in these targets corresponding to increase laser absorption efficiency. The experimental data was supported by PIC simulations.

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Synthesis and compressibility of novel nickel carbide at pressures of Earth outer core

T. Fedotenko[1], S. Khandarkhaeva[1], L. Dubrovinsky[2], K. Glazyrin[3], P. Sedmak[4] and N. Dubrovinskaia[1,5]

[1]Material Physics and Technology at Extreme Conditions, Laboratory of Crystallography, University of Bayreuth, Bayreuth, Germany
[2]Bayerisches Geoinstitut Universität Bayreuth, Bayreuth, Germany
[3] Deutsches Elektronen-Synchrotron, Hamburg, Germany
[4]European Synchrotron Radiation Facility, Grenoble, France
[5]Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden

Knowledge of the abundance and distribution of light elements in the core is fundamental to the understanding of the Earth and other planetary systems. Recent studies on physicochemical properties of Fe carbides at high pressure and temperature conditions show that carbonaceous species of Fe are turned to have a great impact on velocity profile of core-mantle-boundary and outer core [1, 2]. While numerous investigations on Fe carbides at extreme conditions have been conducted, Ni – C system at high PT conditions is still poorly understood. The occurrence of cohenite, $(Fe, Ni)_3C$ which is structurally identical to Fe_3C has been well documented from iron meteorites[3]. However pure cementite type Ni_3C was never reported before.

Here we experimentally investigate the effect of carbon on the elastic properties of nickel at high pressures and temperatures and report a novel high-pressure orthorhombic phase of nickel carbide, Ni_3C with cementite type structure (Pnma, a = 4.519(2), b = 5.801(2), c = 4.009(3)). Ni_3C was synthesized in LH DAC at pressure 180(5) GPa and temperature 3500(200) K through the direct reaction of Ni with carbon from the diamond anvil. The crystal structure of the material at high pressure, its stability and Equation of State were investigated using synchrotron single-crystal X-ray diffraction (ID11 ESRF, P02.2 DESY). We found the Ni_3C to be stable down to 60(2) GPa during the decompression and isothermal equation of state yields a best-fit bulk modulus K0 of 175(11) and K0p of 7.2(6). The calculated from the experimental data bulk sound velocity of a Ni_3C at the Earth outer core conditions gives higher values compare to known iron carbide phases (Fe_3C, Fe_7C3). Thus, taking into account effect of Ni on carbon solubility in Fe-Ni system representing composition of outer core may explain the anomalous elastic properties of the Earth's core

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Ionization and transport in the multi-component plasma of Hot Jupiter atmospheres

Sandeep Kumar[1], Manuel Schöttler, Anna Julia Poser, Uwe Kleinschmidt, Martin French, and Ronald Redmer

Institute of Physics, University of Rostock, D-18051 Rostock, Germany
[1]sandeep.kumar@uni-rostock.de

Ionization and transport in the multi-component plasma of Hot Jupiter atmospheres have been studied. Mass-action laws have been used to calculate the composition of the plasma and electron-ion and electron-neutral transport cross-sections. Based on the plasma composition and these cross-sections, the electrical conductivity, thermal conductivity, and Lorenz number is calculated. The effect of electron-electron scattering on the electrical conductivity, thermal conductivity, and Lorenz number is also studied. The characteristics of ionization and transport with varying mass density and temperature of the plasma are investigated in detail. The profiles of ionization and transport properties in the Hot Jupiter atmospheres by considering different atmospheres models are also studied. Our results are important for understanding Ohmic dissipation and magnetic field generation processes in Hot Jupiters. The method presented here is also useful for the study of ionization, thermodynamics, and transport in other multi-component plasma systems.

A two component model for silicate melt viscosity

D. Langhammer[1], D. Di Genova[1] and G. Steinle-Neumann[1]

[1]Bayerisches Geoinstitut (BGI), Bayreuth, Germany

The viscosity of magmas is an important quantity which controls a range of planetary processes, ranging from the eruptive behaviour of volcanos to the dynamics of a magma ocean. Among all chemical components, volatiles like water have the strongest influence on viscosity.
Modelling the viscous behaviour for different rock types is done by fitting empirical model equations to data sets with different water contents, with the Vogel-Fulcher-Tamman equation (VFT) being most popular. While it generally describes viscosity of magma successful it lacks any physical background, and – in order to account for the impact of water on viscosity – fit parameters are usually extended in an empirical – non-systematic – way.
Here, by contrast, we present a model based on the MYEGA equation by Mauro et al (2009); in contrast to the VFT equation it is based on physical principles and uses infinite temperature viscosity, the glass transition temperature (Tg) and the steepness index as fit parameters. To model the water dependence, we develop a Tg-dependent form of the steepness index m from the MYEGA model: The two component Tg model for polymers of Schneider et al (1997) (S97) is applied.
We fit more than 1000 measurements for 46 different compositions, and find that the combination MYEGA+S97 fits viscosity measurements with comparable if not better quality as publication- and sample-specific VFT models.

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Progress in using XFELs to unravel the superionic character of ice in planetary environments

R. J. Husband[1], H. P. Liermann[1], R. St. McWilliams[2], M. I. McMahon[2]

C. Sanchez-Valle[3], Y. Lee[4]

[1]Deutsches Elektronen Synchrotron, Hamburg, Germany
[2] The University of Edinburgh, Edinburgh, United Kingdom
[3]University of Münster, Münster, Germany
[4]Yonsei University, Seoul, Republic of Korea

Exploration of the phase relations of planetary ices such as H_2O, and its mixtures with other molecular compounds such as ammonia (NH_3) and methane (CH_4) offers insight into the deep interiors of ice planets in the solar system such as Uranus and Neptune, as well as extra-solar planets such as mini-Neptunes [1,2]. However, the creation of the necessary extreme pressure-temperature (P-T) conditions in the diamond anvil cell (DAC) is complicated by the reactive nature of these materials in the superionic and supercritical regimes, where chemical reactions with the sample chamber can ultimately result in confinement failure. Such reactions can potentially be avoided by keeping the sample at elevated temperatures for only very short times and investigating its behavior using short timescale probes such as the femtosecond X-ray pulses produced by X-ray Free Electron Lasers (XFELs). Irradiation with these high-intensity X-ray pulses can also generate extreme temperatures, particularly in the case of high-Z materials, offering the opportunity of performing X-ray heating to access high P-T conditions [3].

In this work, we present the results of preliminary experiments performed at PAL-XFEL at the Pohang Accelerator Laboratory in South Korea, where we used an Au coupler to indirectly heat pure H_2O-ice to superionic P-T conditions. These experiments successfully demonstrated that low-Z materials such as H_2O can be heated though the use of a high-Z coupler. Although the repetition rate of PAL-XFEL (30 Hz) is insufficient for performing X-ray pump-probe experiments (where each subsequent X-ray pulse probes the heated state generated by the previous pulse), we anticipate that the high repetition rate offered by the HED instrument at the European XFEL (4.5 MHz) will allow us to create and probe the superionic state of H_2O and other molecular solids using the rapid succession of 20 fs ultra-short X-ray pulses.

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Structural properties of shock-compressed polyethylene terephthalate

J. Lütgert,[1,2] J. Vorberger,[1] N. J. Hartley,[1,3] K. Voigt,[1] M. Rödel,[1] A. K. Schuster,[1] A. Benuzzi-Mounaix,[4] S. Brown,[3] T. E. Cowan,[1,5] E. Cunningham,[3] T. Döppner,[6] R. W. Falcone,[7,8] L. B. Fletcher,[3] E. Galtier,[3] S. H. Glenzer,[3] A. Laso Garcia,[1] D. O. Gericke,[9] P. A. Heimann,[3] H. J. Lee,[3] E. E. McBride,[3,10] A. Pelka,[1] I. Prencipe,[1] A. M. Saunders,[7] M. Schölmerich,[10] M. Schörner,[3,11] P. Sun,[3] T. Vinci,[4] A. Ravasio,[4] and D. Kraus[1,11]

[1] *Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany*

[2] *Institute for Solid State and Materials Physics, Technische Universität Dresden, 01069 Dresden, Germany*

[3] *SLAC National Accelerator Laboratory, Menlo Park CA 94309, USA*

[4] *LULI, UMR7605, CNRS-CEA, Université Paris VI-Ecole Polytechnique, 91128 Palaiseau Cedex, France*

[5] *Institute of Nuclear and Particle Physics, Technische Universität Dresden, 01069 Dresden, Germany*

[6] *Lawrence Livermore National Laboratory, Livermore CA 94550, USA*

[7] *Department of Physics, University of California, Berkeley CA 94720, USA*

[8] *Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

[9] *CFSA, Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom*

[10] *European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany*

[11] *Institut für Physik, Universität Rostock, 18051 Rostock, Germany*

We present structure measurements of biaxially orientated polyethylene terephthalate (PET, $(C_{10}H_8O_4)_n$, also called mylar) shock-compressed to (155 ± 20) GPa and (6000 ± 1000) K using *in situ* X-ray diffraction. Comparing to density functional theory molecular dynamics (DFT-MD) simulations, a highly correlated liquid at conditions differing from predictions by some equations-of-state (EOS) tables is found, which underlines the influence of complex chemical interactions in this regime. EOS calculations from *ab initio* DFT-MD simulations and shock Hugonitot measurements of density, pressure and temperature confirm the discrepancy to these tables and present an experimentally benchmarked correction to the description of PET as exemplary material to represent the mixture of light elements at planetary interior conditions.

Investigation of hot dense plasmas heated by short-pulse intense laser using x-ray spectroscopy

Xiayun Pan[1, 2], Steffen Sander[3], Michal Šmíd[1], Erik Brambrink[4], Vincent Bagnoud[5], James Colgan[6], Tina Ebert[3], Johannes Hornung[5], Daniel Hartnagel[3], Markus Hesse[3], Thomas Kluge[1], Annika Kleinschmidt[5], Pablo Perez-Martin[1, 2], Amanda Neukirch[6], Katrin Philipp[2], Gabriel Schaumann[3], Alexandra Tebartz[3], Bernhard Zielbauer[5], Markus Roth[3], Katerina Falk[1, 2, 7]

[1] Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany
[2] Technische Universität Dresden, Dresden, Germany
[3] Technische Universität Darmstadt, Darmstadt, Germany
[4] Deutsches Elektronen-Synchrotron, Hamburg, Germany
[5] GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany
[6] Los Alamos National Laboratory, New Mexico, USA
[7] Institute of Physics of the ASCR, Prague, Czech Republic
E-mail: k.falk@hzdr.de

Hot dense conditions in titanium (Ti) targets irradiated with intense sub-picosecond laser pulses on PHELIX laser facility are investigated using x-ray spectroscopy. The effects of microstructured targets on laser absorption and conversion efficiency are studied through the Kα emission. The results are benchmarked by flat titanium foils. Two highly oriented pyrolytic graphite (HOPG) crystal spectrometers are utilized to observe the Kα emission from both front and rear sides of Ti targets. The effective temperature and density of hot dense plasmas are evaluated by analyzing the x-ray spectroscopic data in combination with spectral modelling by SCFLY [1], FLYCHK [2] and ATOMIC [3] codes. Particle-in-cell (PIC) simulations are also implemented to study the evolutionary process of the laser-target interaction, providing time-dependent electron density and energy distribution information, which are used as the inputs of the spectral simulation.

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Investigating the effect of compression rates on the stress development in experiments using the dynamic diamond anvil cell (dDAC) technique.

C. Plueckthun[1,2], N. Giordano[3], R. Husband[3], J. Kaa[1,4], H.-P. Liermann[3], H. Marquardt[5], A. San José Méndez[3], G. Morard[6] and Z. Konôpková[1]

[1]European X-ray Free-Electron Laser Facility GmbH (European XFEL), Schenefeld, Germany, [2]University of Rostock, Rostock, Germany, [3] Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany, [4]TU Dortmund, Dortmund, Germany, [5]University of Oxford, Oxford, England, [6]IMPMC, Sorbonne University, Paris, France

High pressure (P) and temperature (T) experiments using either dynamic (shock, ramp), or static compression techniques play a fundamental role in reproducing the behaviour of matter under extreme conditions relevant to Earth's, or (exo-) planetary interiors and observed by seismic measurements [1,2]. Thereby, common static experiments are limited to long lasting events (e.g. deposition of material, subduction of plates) whilst shock compression experiments simulate very short events (e.g. asteroid impacts), leaving behind a very unexplored field of intermediate strain rates. These intermediate strain rates have become accessible only by means of the newly developed dynamic diamond anvil cell (dDAC) technique [3,4], opening up new P-T pathways to study kinetic phenomena in microsecond –millisecond time scales.

However, difficulties may be encountered in DAC experiments where the sample is compressed uniaxially and non-hydrostatic conditions, hence differential stresses have to be taken into account. Here we present results of fast dDAC compression runs in comparison with quasi-static compression runs (i.e. compression rates below 1 GPa/s) with and without pressure transmitting media. We performed micro-strain evolution analysis of different standard materials such as Au, Pt, MgO with cubic crystalline symmetry, as well as we investigated the structural behaviour of Re, Fe with hexagonal closed-packed (hcp) symmetry and determined the c/a ratio evolution as a function of pressure, as main indicators of the onset of non-hydrostaticity [5-7]. The current results highlight the importance to determine the effect of stress development in dDAC experiments.

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Atomic-scale insight into the material properties of liquid iron alloys as a function of pressure, temperature, and composition

E. S. Posner and G. Steinle-Neumann

Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth

The material properties of iron alloys under extreme pressure (P) and temperature (T) conditions are required to understand the origin, dynamics, and evolution of planetary cores. We combine first-principles molecular dynamics simulations with laboratory experiments to systematically determine the atomic-scale mechanisms that control the equilibrium, elastic, and transport properties of liquid iron alloys as a function of pressure, temperature, and composition. Our previous results revealed a strong relationship between atomic size and transport behavior in binary liquid iron alloys, which provides a means to predict one property if the other is known. We now extend the study to ternary and higher-component liquid iron alloys using a topological model that provides insight into the material properties of more realistic planetary core compositions. Our results demonstrate the mechanisms by which nickel and sulfur modify the short-range order of liquid iron, which affects the chemical equilibrium and transport properties of iron and other alloying elements, as reported in previous high P-T experiments.

Metallization of dense fluid helium from ab initio simulations

Martin Preising[1], Ronald Redmer[1]
[1]*Universität Rostock, GERMANY*

ABSTRACT.

An earlier study [1] benchmarked Density Functional Theory (DFT) coupled with classical Molecular Dynamics (MD) with all available experimental data on dense helium in recent years. A subsequent study [2] calculated the helium melting line with DFT-MD. These two studies allows for the examination of the metallization of fluid helium consistently with DFT-MD.

We study the insulator-to-metal transition at densities between 1 and 22 g/cm^3 and temperatures between 10 000 and 50 000 K. We calculate the equation of state, the band gap dependent on density and temperature by using different definitions [3-6], the DC conductivity, the reflectivity, and the ionization degree for which a novel method has been proposed recently [see M. Bethkenhagen et al., Phys. Rev. Res. 2, 023260 (2020)].

We find no indication of a first-order phase transition in any of the properties studied here and conclude that the metallization of fluid helium is continuous. For instance, we do not observe jumps in the DC conductivity and/or the reflectivity when the band gap closes. However, the ionization degree increases from below 10% at the lowest to over 99% at the highest densities which reflects the continuous insulator-to-metal transition. The increase is almost exclusively driven by pressure ionization and shows only a weak temperature dependence.

We discuss the high-pressure phase diagram of helium and the implications of our results on the structure of astrophysical objects like gas giant planets and brown dwarfs.

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Influence of a thermal boundary layer on the thermal evolution of Uranus and Neptune

L. Scheibe[1], N. Nettelmann[2] and R. Redmer[1]

[1]Institut für Physik, Universität Rostock, Albert-Einstein-Str. 23-24, D-18059 Rostock, Germany

[2] Institut für Planetenforschung, DLR, Rutherfordstraße 2, D-12489 Berlin, Germany

It has been a long-standing challenge to reconcile the perceived similarities of Uranus and Neptune with their highly different intrinsic heat fluxes. Previous evolution calculations using the conventional assumption of an adiabatic interior yield too high present-day luminosities or - equivalently - too long cooling times for Uranus (e.g. [1,2]). For Neptune, however, we found that similar assumptions yield too short cooling times [3].

One proposed mechanism for reproducing the observed brightness is a conducting interface between the hydrogen- and helium-rich outer part and the ice-rich inner part that would inhibit efficient energy transport across it [4]. In this work, we use our recently developed tool for modelling giant planets based on the Henyey-method for stellar evolutions [5] to investigate such a conducting interface in the planet's interior, examining the influence of parameters such as assumed layer thickness and thermal conductivity on the cooling behaviour.

We find that even a thin conductive interface of a few kilometers has significant influence on the planetary cooling. Initially, the presence of such a boundary layer speeds up cooling, while after about 0.1-0.5 Gyr the cooling is slowed down drastically compared to the adiabatic case, similar to what was found for Saturn previously [6]. Our preferred solutions for Uranus suggest equilibrium evolution with the solar incident flux, while for Neptune, we find that plateaus in effective temperature near its observed value require fine-tuned combinations of layer thickness and thermal conductivity. For both planets our models suggest that they have reached a state where their luminosity stays nearly constant due to loss of primordial heat from the deep interior, and that they are warm and fluid inside.

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Ab initio analysis of x-ray Thomson scattering

M. Schörner[1] and R. Redmer[1]

[1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany

We demonstrate a state-of-the-art approach for calculating x-ray Thomson scattering spectra from DFT-MD simulations based on a modified Chihara formula.
We compute the ionic contribution from the ion-ion structure factor and the total form factor of the electrons, while utilizing the fluctuation-dissipation theorem to predict the inelastic response of the electron system including free-free, bound-free, and bound-bound transitions.
As the inelastic contribution is only directly accessible in the long wavelength limit, we extend it to finite wave vectors by using the Mermin formalism with dynamic collision frequencies determined with DFT-MD.
Our results are compared to the Born-Mermin approach employed by most codes that analyse x-ray Thomson scattering experiments at various temperatures and densities in the WDM regime.

$MgSiO_3$-SiO_2 eutectic at lower mantle pressure from multi-anvil experiments

J. Yao[1], G. Steinle-Neumann[1], D. J. Frost[1]

[1]Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany

Giant impact events in the early Earth have led to large-scale melting, potentially up to the entire planet being molten. Crystallization of silicate melt from the magma ocean – or in residual reservoirs provides an important constraint on the chemical differentiation and stratification in the Earth. The MgO-SiO_2 system serves as the first-order approximation to mantle composition, and melting relations along this join informs us about the crystallizing sequence in the magma ocean.

A lot of work has focused on the MgO-rich side of this join (MgO-$MgSiO_3$) with many model compositions of both the modern and primordial mantle being in that range in terms of MgO/SiO_2 ratio. However, for a full description of thermodynamics in the MgO-SiO_2 system, the SiO_2-rich side also needs to be considered. We have performed a multi-anvil experiment for $Mg_{0.4}Si_{0.6}O_{1.6}$ at 24 GPa and 2700 K using a 7/3 cell assembly and rhenium capsule in the Sumitomo press at BGI. The run product is analyzed with the scanning electron microscope for texture and with the electron microprobe for chemical composition. Quenched stishovite is visible, coexisting with the liquid; large stishovite crystals have settled at the bottom of the capsule and the liquid evolves towards a silica poorer composition compared to the starting material ($xSiO_2$=0.60). The liquid composition is determined with $xSiO_2$=0.53(±0.03), tightly constraining the eutectic.

Based on the chemical analysis of the residual melt, the MgO-SiO_2 phase diagram is calculated at 24 GPa and extrapolated to the core mantle boundary (136 GPa) by using the equality of the chemical potential between solid and liquid phases coexisting at the two eutectic points, constraints on the melting temperature of the liquidus phases and thermodynamic models and parameters of the minerals involved from the literature.