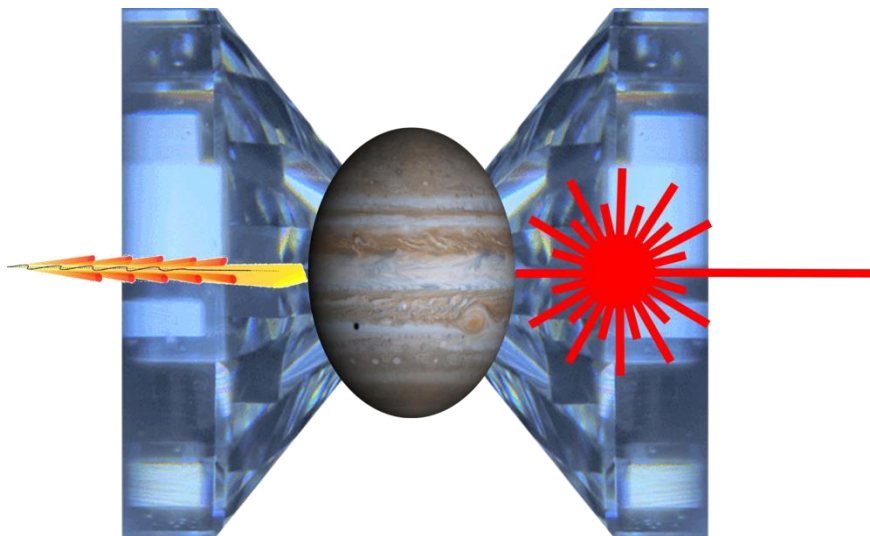


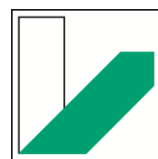
4th Joint Workshop on High Pressure, Planetary and Plasma Physics

(4HP4)

September 23-25, 2015



Bayerisches Geoinstitut
Universität Bayreuth



UNIVERSITÄT
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Location

Universität Bayreuth
Bayerisches Geoinstitut
Universitätsstr. 30 (Infopunkt 5)
95447 Bayreuth
Germany
49°55′37″(N), 11°35′12″(E)

Lectures are held in the AI building, lecture hall H33.

Coffee breaks, laboratory tours and the poster session are held in the BGI foyer (2nd floor).

Maps of the Campus and the city can be found at the end of this program brochure.

Preface

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

- Generation of such conditions at FLASH and at 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) through advances in the multi-anvil and diamond anvil cell techniques.
- A combination of static and dynamic compression devices.
- Development of new diagnostic tools.
- Predictions of high pressure and temperature properties of materials from ab-initio methods. Advances in methods and computer technology provide an increasing number of predictive data set for planetary interiors.
- Application of such results to the study of the interior structure and dynamics of planetary and astrophysical bodies.

To bring together researchers from these diverse fields in the physical sciences a workshop series has been established by DESY, XFEL, DLR Berlin, the University of Rostock and Bayerisches Geoinstitut (BGI). Earlier workshops were held at DESY in Hamburg (2012), at DLR Berlin (2013) and at the University of Rostock (2014). Planning is already underway for the 2016 workshop, to be held again in Hamburg. For the 4th annual workshop on high pressure, planetary and plasma physics (4HP4) we have put together seven scientific sessions with contributions from all of the fields mentioned above:

- I. Warm dense matter and plasmas
- II. Diagnostics of dense plasmas
- III. Giant planets
- IV. Earth's core
- V. High pressure physics
- VI. Planetary mantles
- VII. Small planetary bodies

Due to the emphasis of research at BGI the 4HP4 program is more heavily weight towards the interior of the Earth and other planets in our solar system. This reflects the experience from the previous workshops where research performed at the organizing partner has always been at the center of attention. In the past, the shifting focus has been a welcome opportunity to widen the perspective of participants and discussions – and we hope that the current workshop continues along this line.

Bayreuth, September 18, 2015

Gerd Steinle-Neumann.

Technical Details

Poster Session

The poster session is held in the foyer of the BGI building (2nd floor). It is scheduled for Monday late afternoon. Beer (as well as other beverages) and pretzels will be served. The poster boards will be up and accessible for the entire workshop such that discussion around posters is also possible at other times.

Internet Access

Wireless internet is available at both locations of the workshop (AI and BGI buildings). Access is either through eduroam or individual logins and passwords. Login/password pairs are personal and can be obtained in exchange for a signature at registration.

Coffee Breaks

Coffee, drinks, cookies and fruit will be served during the breaks between the oral sessions in the BGI foyer, i.e., across the street from the lecture hall.

Lunch

Light lunch will be provided on Wednesday in the BGI foyer. For lunch on Thursday and Friday the University cafeteria (Mensa) is available to workshop participants. The cafeteria operates cash-free, and charged guest cards (4 EUR deposit + 6 EUR balance) are available at the registration desk or from of the organizers for 10 EUR. These cards can be returned at refund stations in the Mensa. You can ask one of the local organizers for further help.

The sandwich place (Fine Toast) that caters lunch on Wednesday is within easy walking distance from Campus (see map). Other options in the city are too far for convenient lunch.

Conference Dinner

There will be the opportunity to participate at a conference dinner on Thursday (7:30pm) at the restaurant "Goldener Löwe" (see map). At the registration desk menu choices and prices are available. Please indicate if you want to participate at the dinner and mark your choice by Thursday noon. Goldener Löwe is located directly on the bus line from the University (bus number 306 towards "Roter Hügel", bus stop "Kulmbacher Strasse") and easy to recognize by the golden lion that lies in front of it. The bus leaving the stop "Mensa" on Campus at 6:56pm will reach "Kulmbacher Strasse" at ~7:15pm. The restaurant is within easy walking distance from the downtown area and most of the hotels.

Laboratory Tours

On Thursday afternoon there is the opportunity to participate in laboratory tours. The tours will be to four different laboratories (1/2 hour each) in relatively small groups and be guided by experienced researchers:

- Multi-anvil presses
- Deformation laboratory
- Diamond-anvil cells
- Transmission electron microscopy

The tours also provide an opportunity for discussion. At registration please indicate whether you would like to participate in the lab tours.

If you are interested in other laboratories or you want to talk to other scientists at BGI, the local organizers will try to arrange such meetings/opportunities.

HIBEF Meeting

The seminar room on the 3rd floor of the BGI building is reserved for the Wednesday evening starting at 6:00pm.

Invited Speakers

Frédéric Datchi, IMPMC, Université Pierre et Marie Curie, Paris, France.

Leonid Dubrovinsky, Bayerisches Geoinstitut, University of Bayreuth, Germany.

Gregor Golabek, Bayerisches Geoinstitut, University of Bayreuth, Germany.

Scott King, Virginia Institute of Technology, Blacksburg, VA, United States.

Stewart McWilliams, University of Edinburgh, United Kingdom.

Giulio Monaco, Università degli Studi de Trento, Italy.

Guillaume Morard, IMPMC, Université Pierre et Marie Curie, Paris, France.

Conference Program

Wednesday, September 23			Location
12:00	Registration and light lunch		BGI
13:45	Steinle-Neumann	Opening	AI
Session I: Warm Dense Matter and Plasmas Convener: Ronald Redmer			AI
14:00	McWilliams	Warm dense matter on the desktop: Miniaturizing dynamic extremes experiments	
14:30	Gericke	Ionisation Equilibrium in Dense Matter	
14:50	Bethkenhagen	Molecular mixtures at high pressures	
15:10	Zastrau	Exploring dense plasmas at X-ray free electron lasers	
15:30	Coffee break		BGI
Session II: Diagnostics of Dense Plasmas Convener: Alessandra Benuzzi Mounaix			AI
16:00	Monaco	Ion acoustic waves in warm dense matter	
16:30	Appel	Experimental platform for Inelastic X-ray Scattering at the HED science instrument at the European XFEL	
16:50	Redmer	Dynamic ion-ion structure factor in warm dense matter	
17:10	Recoules	Experimental and ab initio investigations of microscopic properties of laser-shocked Ge-doped CH ablator	
17:30	Poster Session Beer and brezels	HIBEF Meeting (18:00, BGI 4.2.03)	BGI

Thursday, September 24			Location
Session III: Giant Planets Convener: Frank Sohl			AI
9:00	Datchi	Simple molecules at planetary conditions: some recent results	
9:30	Nettelmann	Giant planet luminosities, models, and constituent physics	
9:50	Duarte	A parameter study of Jupiter-like dynamo models	
10:10	Kellermann	Modeling interior structures of rocky exoplanets using different equations-of-state	
10:30	Coffee break		BGI
Session IV: Earth's Core Convener: Gerd Steinle-Neumann			AI
11:00	Morard	Study of liquid iron alloys under extreme conditions	
11:30	Wagle	Conductivity of iron along its melting curve	
11:50	Mattesini	Candy Wrapper for the Earth's Inner Core: Bridging Mineral Physics and Seismological Observations	
12:10	Wicht	Explaining lateral differences in inner core structure	
12:30	Lunch break		
Session V: High Pressure Physics Convener: Karl Syassen			AI
14:00	Dubrovinsky	Equations of state of metals from X-ray diffraction data at static pressures above 5 Mbar	
14:30	Guthrie	Neutron science in the megabar regime	
14:50	Schöttler	Free energy model for the high pressure solid phases of carbon	
15:10	French	Construction of a thermodynamic potential for the water ices VII and X	
15:30	Coffee break		BGI
16:00	Laboratory Tours: Multi-Anvil Presses Diamond Anvil Cells Deformation Transmission Electron Microscopy		BGI
19:30	Conference Dinner at Restaurant Goldener Löwe		

Friday, September 25			Location
Session VI: Planetary Mantles Convener: Frank Sohl			AI
9:00	King	Mantle Rheology: Exploring Laboratory and Geophysical Constraints	
9:30	Marquardt	Strength of (Mg,Fe)O ferropericlaste at high-pressures and high-temperatures and slab stagnation in the shallow lower mantle	
9:50	Cebulla	High pressure phase diagram of MgO and FeO	
10:10	Petitgirard	Fate of silicate melts at core-mantle boundary conditions	
10:30	Coffee break		BGI
Session VII: Small Planets Convener: Attilio Rivoldini			AI
11:00	Golabek	Early thermomechanical evolution of planetesimals	
11:30	Posner	High P-T diffusion experiments in liquid iron	
11:50	Plesa	Depth-dependence of viscosity and its influence on the Martian mantle dynamics	
12:10	Rückriemen	The curious case of Ganymede's magnetic field	
12:30	Steinle-Neumann Liermann	Concluding Remarks	AI

List of Posters	
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Appel	An upcoming facility for experimental studies of high-energy density states of matter: the HED science instrument at the European XFEL
Baetz	The HIBEF user consortium
Papagiannouli	Non-resonant Frequency-domain Interferometry for Probing the Phase Transitions of Silicon
Evans	Time-resolved studies of phase transition dynamics
Konopkova	Thermal conductivity measurements in metals at high pressure and temperatures
Liermann	Conceptual Design of the DAC setup for dsDAC and dDAC experiments at the HED instrument of the European XFEL
Mueller	Novel LVP Techniques
Ovsyannikov	Properties of metastable high-pressure polymorphs of manganese oxides
Ovsyannikov	High-pressure high-temperature synthesis of bulk $\text{Si}_{1-x}\text{B}_x$ alloys: two semiconductors form an unusual metal
Bolis	Investigation of the Magnesium Oxide phase diagram
Bouchet	Calculations of phonon spectra from ab-initio MD simulation
Rivoldini	Mercury's thermal evolution and core crystallisation regime
King	Geodynamics of Mercury: MESSENGER spacecraft observations, equation of state, and rheology constraints
Chust	Crystallizing the Martian Magma Ocean
Csizmadia	Observability of shape distortion of exoplanets with future space observatories

Abstracts of Talks and Posters

1.1 Wednesday 23.Sept.15 14:00 (invited)

Warm dense matter on the desktop: Miniaturizing dynamic extremes experiments

Stewart McWilliams

Centre for Science at Extreme Conditions, School of Physics and Astronomy, University of Edinburgh

The laboratory study of matter at extremes of pressure, temperature, and density often suffers from the significant size and cost of facilities needed to generate extreme conditions. The laser-heated diamond anvil cell offers an alternative, bench-top route to extreme pressures and temperatures, which has recently seen dramatic growth in accessible conditions. In this talk I will discuss recent efforts to produce and characterize extreme states of hydrogen, helium, and other materials using a dynamically laser-heated diamond cell. The conditions studied have previously been accessible only via dynamic compression at large facilities, or have never before been explored. Novel optical measurements, unique thermodynamic pathways, and sustained confinement of warm dense states are demonstrated. Central questions regarding the nature of insulator-metal transitions in warm dense matter, long studied by theorists, are addressed experimentally for the first time using these novel approaches.

1.2 Wednesday, 23.Sept.15, 14:30

Ionisation Equilibrium in Dense Matter

D.O. Gericke and R.A. Baggott

University of Warwick

The properties of dense matter in large planets and other compact objects are often strongly influenced by the ionization degree. Although free and bound states can't be defined clearly, concepts like an effective ionization energy allow to transfer many theoretical approaches into a regime with strong interactions and degenerate electrons. Recent experiments have shown significant shortcomings in the standard modelling of the ionization equilibrium and, indeed, even contradictory results. The talk will give an overview over simulation and other theoretical approaches to account for medium in dense matter and further extent these concepts. The improved model accounts for nonlinear screening, the changes due to remaining bound states, weak correlation effects, and quantum degeneracy. Modelling of the influence of different bound states has been found very important to meet experimental data as well as to resolve the, seemingly, contradicting results of different experiments. A final outlook to nonequilibrium systems will conclude the talk.

1.3 Wednesday, 23.Sept.15, 14:50

Molecular mixtures at high pressures

Mandy Bethkenhagen,¹ Edmund R. Meyer,² Daniel Cebulla,¹ Sebastien Hamel,³ Christopher Ticknor,² Lee A. Collins,² Joel D. Kress,² and Ronald Redmer¹

¹*Universität Rostock, Institut für Physik, 18057 Rostock, Germany*

²*Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

³*Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

The interiors of the giant planets Uranus and Neptune are dominated by a mixture of the molecular compounds water, ammonia and methane. Many observable properties of these planets, such as luminosity, gravitational moments and magnetic fields, 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]

In particular, the superionic phases of water and ammonia, characterized by highly mobile hydrogen ions diffusing through a lattice of oxygen and nitrogen ions, respectively, have gained much attention. For water, the influence of such a phase on the properties of the giant planets as well as on exoplanets has been discussed widely [2,3], while it is an open question how the properties of such a water layer change when other compounds are introduced.

To address this question we performed ab initio simulations based on density functional theory using the VASP code [4] for a variety of molecular mixtures starting with a 1:1 water-ammonia mixture. Heating up structures which we had found from evolutionary random structure search calculations with XtalOpt [5] we find superionic water-ammonia structures present up to several Mbar. Adding methane to the water-ammonia mixtures we observe amorphous structures of nitrogen and oxygen while carbon forms short chains. Evaluating the equation of state and structural properties such as diffusion coefficients and bond autocorrelation functions for varying mixing ratio we discuss general trends with respect to the N:O:C concentration. The obtained results are essential to construct new interior models for Uranus and Neptune as well as Neptune-like exoplanets. [6]

References:

- [1] R. Chau, S. Hamel and W. J. Nellis, *Nature Communications* 2, 203 (2011).
- [2] R. Redmer, T.R. Mattsson, N. Nettelmann and M. French, *Icarus* 211, 798 (2011).
- [3] L. Zeng and D. Sasselov, *Astrophysical Journal* 784, 96 (2014).
- [4] G. Kresse and J. Hafner, *Physical Review B* 47, 558 (1993).
- [5] D. C. Lonie and E. Zurek, *Computer Physics Communications* 182, 372 (2011).
- [6] N. Nettelmann, R. Helled, J. J. Fortney and R. Redmer, *Planetary and Space Science* 77, 143 (2013).

1.4 Wednesday 23.Sept.15, 15:10

EXPLORING DENSE PLASMAS AT X-RAY FREE ELECTRON LASERS

U. Zastra¹, M. Nakatsutsumi¹, K. Appel¹, A. Pelka², G. Priebe¹, A. Schmidt¹, I. Thorpe¹, C. Baehtz², T. Cowan², and Th. Tschentscher¹

¹*European XFEL, Hamburg, Germany*

²*Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany*
and the HIBEF user consortium (www.hibef.de)

The advent of the first free-electron X-ray lasers (XFELs), FLASH in 2004 and LCLS in 2009, may prove to be the most profound development since the invention of the laser and, equally, the synchrotron. Sharp improvements in a number of laser parameters, most notably intensity and pulse duration, support this expectation. This brings scientific dreams within reach. Indeed, the unprecedented opportunities and expectations have triggered considerable research activities worldwide. The talk will yield an overview of the experimental application of today's XFELs to explore matter in extreme conditions with advanced x-ray spectroscopy.

In the near future, the High Energy Density Science (HED) instrument at the European X-ray Free-Electron Laser Facility in Hamburg, Germany, will allow investigations of an even wider range of materials and systems at extreme conditions. For sample excitation a variety of high energy drivers will be installed [1]. In particular, three separate optical laser systems will be available for warm- to hot-dense-matter creation, dynamic compression and laser-plasma interaction in electron-relativistic regime. These drivers will allow studying various phase space parameters with time-resolution down to 10 fs, pressures into the TPa regime, and electric field strength up to 1020 W/cm. This unique instrument is designed to enable the application of various x-ray probes including spectroscopic, diffraction and imaging methods [2]. It will operate in the photon energy range from 3 to above 20 keV and will feature a variety of platforms facilitating the usage of different techniques in user-driven experiments. Future capabilities of the HED instrument, including the contributions from the Helmholtz International Beamline for Extreme Fields (HIBEF [3]) will be presented along with selected science cases.

[1] M. Nakatsutsumi, K. Appel, G. Priebe, I. Thorpe, A. Pelka, B. Muller, Th. Tschentscher, Technical design report: Scientific instrument High Energy Density Physics (HED), XFEL:EU TR-2014-001, Germany, 196 p (2014). doi:10.3204/XFEL.EU/TR-2014-001. See also www.xfel.eu/research/instruments/hed

[2] K. Appel, M. Nakatsutsumi, A. Pelka, G. Priebe, I. Thorpe, Th. Tschentscher, Plasma Phys. Control. Fusion 57, 014003 (2015).

[3] www.hibef.de

2.1 Wednesday, 23.Sept.15, 16:00 (invited)

Ion acoustic waves in warm dense matter

G. Monaco¹, T. White², G. Gregori², N. Hartly², L. Fletcher³, K. Appel⁴, T. Tschentscher⁴, D. Chapman⁵, D.O. Gericke⁵, T. Doeppner⁶, H-J. Lee⁷, B. Nagler⁷, E. Galtier⁷, E. Granados⁷, U. Zastrau⁷, P. Heinmann⁷, A. Schropp⁷, S.H. Glenzer⁷, J. Hastings⁷

¹*Physics Department, University of Trento, I.*

²*Physics Department, University of Oxford, UK.*

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⁴*European XFEL, Hamburg, D.*

⁵*Physics Department, University of Warwick, UK.*

⁶*SLAC, Menlo Park, CA, USA.*

⁷*LLNL, Livermore, CA, USA.*

Recent results obtained using FEL-based high resolution inelastic x-ray scattering to probe the ion acoustic waves in warm dense Al are here presented. An about twofold compression of Al at a temperature of ~ 2 eV has been reached using two counter-propagating shock waves generated by two 3 ns long, 5 J laser beams at the MEC beamline at LCLS. A high-resolution spectrometer based on a diced crystal analyzer operated in close to backscattering at the Si(4,4,4) reflection has been setup to reach a total energy resolution of ~ 100 meV. This has allowed resolving a Brillouin spectrum for an exchanged wavevector of 2.1 \AA^{-1} . The experimental results are here discussed in terms of density functional simulations.

2.2 Wednesday, 23.Sept.15, 16:30

Experimental platform for Inelastic X-ray Scattering at the HED science instrument at the European XFEL

K. Appel¹, G. Monaco², M. Nakatsutsumi¹, H. Sinn¹, I. Thorpe¹, Th. Tschentscher¹ and U. Zastra¹

¹European XFEL, Hamburg, Germany

²University of Trento, Trento, Italy

Free-electron laser facilities enable new applications for short-term processes like the response of dynamical excitations. One key application in the high-energy density regime is the study of the dynamic structure factor as it allows to retrieve electron and ion temperatures in warm and hot dense matter on a short time scale. Inelastic X-ray Scattering (IXS) at a self-seeded XFEL has been proven to be a suitable method to determine the ion-acoustic waves in a plasma (G. Monaco, in prep.).

At the HED instrument, IXS will be one of the key x-ray techniques to be implemented in the main interaction area [1]. The repetition rate for the set-up is matched with the repetition rate of the high power optical lasers, which is 10 Hz at maximum. Besides a high photon flux, the critical parameter for IXS experiments is the achievable spectral resolution: while for the study of electron distributions a $\Delta E/E$ of 10^{-3} - 10^{-4} (10^{-1} eV at 10 keV) is sufficient, the study of ion distributions requires a $\Delta E/E$ of 10^{-5} - 10^{-6} (100 meV - 10 meV at 10 keV). At the HED science instrument, an overall instrument resolution of better 80 meV down to 25 meV is planned using Si₄₄₄ and Si₅₅₅ reflections for both the monochromator and the analyser. Self-seeding will be available at SASE2 from early HED operation on and will ensure a sufficient flux at the sample and a $\Delta E/E$ of about 10^{-4} - 10^{-5} . A high-resolution monochromator in backscattering geometry will be installed far upstream in the tunnel to reduce the bandwidth by a factor of 10. For the moment, the higher order reflections of Si₁₁₁ are foreseen but a later exchange to cuts without higher harmonic contributions is feasible. For Si₄₄₄ and Si₅₅₅, the energies close to back reflection are 7902.5 eV and 9897.5 eV with intrinsic widths of 40 and 15 meV, respectively. The monochromatic beam can be focused to 10 -20 μm on the sample using a downstream set of compound refractive lenses with a focal length of more than 100 m. The installation of the focusing optics downstream of the monochromator will ensure a high momentum instrument resolution. The sample vacuum chamber is sufficiently large to allow the installation of a spherical analyser crystal at a distance of 1 m from the sample. Here, it is planned to install diced crystals in forward (5 - 20°) and backscattered (140°) orientations to make the Q-dependence of the dynamic structure factor accessible. With the envisaged set-up, Q-values between 0.35 - 1.40 \AA^{-1} and 7.54 \AA^{-1} using Si₄₄₄ and 0.44 to 1.74 \AA^{-1} and 9.43 \AA^{-1} using Si₅₅₅ will be made accessible. For the analyser in forward direction, scanning will be enabled by the use of motorized curved rails.

In this contribution, we present the actual layout of the foreseen experimental facility for IXS including the x-ray parameters, the high-resolution monochromator, the experimental set-up, detectors and the optical excitation sources.

References

[1] M. Nakatsutsumi, K. Appel, G. Priebe, I. Thorpe, A. Pelka, B. Muller, Th. Tschentscher, Technical design report: Scientific instrument High Energy Density Physics (HED), XFEL:EU TR-2014-001, Germany, 196 p (2014). doi:10.3204/XFEL.EU/TR-2014-001. See also www.xfel.eu/research/instruments/hed

2.3 Wednesday, 23.Sept.15, 16:50

Dynamic ion-ion structure factor in warm dense matter

Hannes R. Rüter*, Bastian Witte and Ronald Redmer

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**Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany*

We perform ab initio simulations based on finite-temperature density functional theory in order to determine the static and dynamic ion-ion structure factor for warm dense Li, Be and Al, see [1] for details of the method. We calculate the dynamic structure factor via the intermediate scattering function and extract the dispersion relations for the collective excitations. We present a generalized hydrodynamic model which is used to fit the numerical data. First, we benchmark our calculations against experimental data in the liquid metal domain. Second, we predict the dynamic ion-ion structure factor and related quantities for the warm dense matter regime and compare with results of approximate theoretical methods. The new results can be checked in experiments using narrow-bandwidth free electron laser radiation available at, e.g., LCLS in Stanford and the future European XFEL in Hamburg.

[1] H.R. Rüter and R. Redmer, Phys. Rev. Lett. 112, 145007 (2014).

2.4 Wednesday, 23.Sept.15, 17:10

Experimental and ab initio investigations of microscopic properties of laser-shocked Ge-doped CH ablator

G. Huser¹, V. Recoules¹, N. Osaki^{2,3}, T. Sano⁴, Y. Sakawa⁴, G. Salin¹, B. Albertazzi², S. Iketani², M. Kita², T. Ogawa², Y. Sato², R. Kodama^{2,3}

¹*CEA, DAM-DIF, Bruyères le Chatel, Arpajon*

²*Graduate school of Engineering, Osaka University, Osaka, Japan*

³*Photons Pioneers Center, Osaka University, Osaka, Japan*

⁴*Institute of Laser Engineering, Osaka University, Osaka, Japan*

Plastic materials doped with mid-Z elements are used as ablaters in Inertial Confinement Fusion (ICF) capsules and in their surrogates. Several laser experiments have been done on polystyrene, CH foams or glow discharge polymer and have provided measurements of the principal Hugoniot curve as well as shock front reflectivity. In parallel, Ab Initio Molecular Dynamics (AIMD) simulation is used to produce Equation of States (EoS) and transport properties of CH on a large pressure-temperature domain. All this studies were mainly focused on pure CH. On this poster, Hugoniot EoS and electronic properties of CH doped germanium (at 2.5% and 13% dopant fractions) are investigated experimentally up to 7Mbar using velocity and reflectivity measurements of shock fronts on the GEKKO laser at Osaka University. Theoretical investigation of Hugoniot pressure and reflectivity is also performed using AIMD with ABINIT code in the framework of density functional theory. A special care is needed to perform such kind of simulation with masses highly different among the species. Theoretical results are compared to tabulated EoS used in hydrocode and to the experimental results.

3.1 Thursday, 24.Sept.15, 9:00 (**Invited**)

Simple molecules at planetary conditions: some recent results

Frédéric Datchi

IMPMC, Sorbonne Universités/Université Paris 6, CNRS, IRD, MNHN, 4 place Jussieu, 75005 Paris, France

Models of the giant planets mostly rely on our knowledge of a few simple molecules under extreme P-T conditions. For Neptune and Uranus, the existence of a thick layer of ice (a mixture of water, ammonia and methane), located between a small rocky core and a thin gaseous atmosphere, is generally assumed. Pressure and temperature conditions in this ice layer range from about 10 GPa and 2000 K up to 700 GPa and 6000 K. The properties of these planets are thus expected to be largely influenced by the behavior of these ices under extreme P-T conditions. In particular, the ice layer is suspected to be the source of the non-dipolar, non-axisymmetric magnetic fields measured by the Voyager II spacecraft. This magnetic field is believed to originate from the dissociation of the water molecules into ionic species at high P/T, which is supported by several first-principles calculations predicting the ionization of water both in the fluid and solid phases. Dissociation of water ice has been inferred from a number of experiments, although a direct proof is still lacking. Furthermore, the presence of other molecules, in particular ammonia and methane, in the ice layer has so far been largely neglected, and it is not known how they influence its properties.

Here I will present the results of our investigations on pure ammonia and water/ammonia mixtures from static high P-T experiments and computer simulations. Pure ammonia is found to transform into an ionic crystal at low temperatures (300 K) above 150 GPa [1], and to a superionic solid above 60 GPa at high temperatures (750 K) [2], in good agreement with DFT predictions. In water/ammonia mixtures of 1:1 composition (ammonia monohydrate), the presence of the OH^- and NH_4^+ ionic species is detected at pressures as low as 7 GPa in the solid phase [3], but the compound does not fully ionize contrarily to what DFT predicts. Furthermore, the equation of state is found to deviate from the ideal mixing rule above 40 GPa.

I will also present our current efforts to study light molecular liquids under extreme conditions using synchrotron x-ray diffraction and illustrate with recent results on fluid H_2 [4] and CO_2 [5].

[1] S. Ninet, F. Datchi, P. Dumas, M. Mezouar, G. Garbarino, A. Mafety, C. J. Pickard, R. J. Needs and A. M. Saitta. *Phys. Rev. B* 89, 174103 (2014)

[2] S. Ninet, F. Datchi and A. M. Saitta. *Phys. Rev. Lett.* 108, 165702 (2012)

[3] C. Liu et al, in prep.

[4] G. Weck, G. Garbarino, P. Loubeyre, F. Datchi, T. Plisson, and M. Mezouar. *Phys. Rev. B* 91, 180204(R) (2015)

[5] F. Datchi, G. Weck, A. M. Saitta, Z. Raza, G. Garbarino, S. Ninet, D. K. Spaulding and M. Mezouar, submitted

3.2 Thursday, 24.Sept.15, 9:30

Giant planet luminosities, models, and constituent physics

N. Nettelmann, R. Püstow, R. Redmer

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The giant planets in the solar system are visible by eye as they reflect the sunlight. Moreover, they are self-luminous at IR wavelengths, an important property that yields insight into their internal structure. However, Uranus and Saturn challenge our understanding of giant planets: Uranus is very faint, like Earth, whereas Saturn appears to be too luminous. While the origin of Uranus' faintness may be related to the physics of ices and rocks under high pressures, Saturn's brightness could be a result of H/He phase separation under compression.

Here we use the examples of Uranus, Saturn, and Jupiter to discuss models for giant planet internal structure and evolution. The models are built on astrophysical observational constraints, theoretical properties of matter under high pressures, physical principles, and simplifying assumptions. In particular, we show that Uranus' faintness can be explained by the assumption of a thermal boundary layer with inefficient diffusion of heat and particles across. For Uranus we propose a warm, ice/rock-rich interior where rocks are miscible with the dissociated ices as illustrated in Figure 1. Our new models for Jupiter and Saturn make explicit use of ab initio simulations based H/He phase diagrams and associated helium rain to explain their luminosity.

Finally, we outline parameter spaces for future laboratory measurements that could further help to validate and improve the planet models.

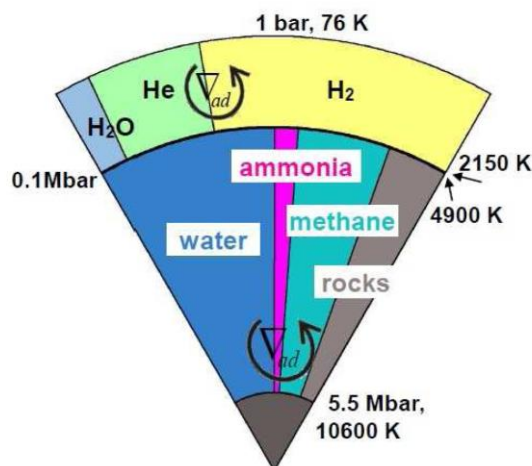


Figure 1: Uranus structure model with thermal boundary layer. This new model is consistent with the observed low luminosity and the gravity field. It suggests miscibility between warm dense ices and rocks.

3.3 Thursday, 24.Sept.15, 9:50

A parameter study of Jupiter-like dynamo models

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The upcoming missions to Jupiter will provide new information about the outer flow dynamics and magnetic field of the planet. In the last few years, the interest in more accurate numerical models of the planet significantly increased and remarkably close models have been published which incorporate interior radial profiles obtained from ab initio equations of the interior of the planet. The solutions of these numerical models for the dynamics already show several surface features that closely reproduce the observational data available in the present. The future observational data will provide better constraints for numerical models, thus allowing comparisons at a much higher degree. In the meantime, the next step in the numerics is to develop parameter studies, which will provide us a broader range of models incorporating Jupiter's interior profiles. Simplifications are necessary when it comes to numerical modelling and so we present here an extensive parametric study of Jupiter models, alongside other previously published polytropic models for comparison, where different Ekman numbers and Prandtl numbers at different supercriticalities are tested and presented. Furthermore, for a more detailed analysis we focus on different heating mechanisms and Jupiter-like density and electrical conductivity gradients. The density gradient is fixed for the Jupiter models, but the steep electrical conductivity profile cannot be achieved for a nearly full interior model (up to 1% below the surface) due to the limitations of current computational resources.

3.4 Thursday, 24.Sept.15, 10:10

Modeling interior structures of rocky exoplanets using different equations of state

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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. Simultaneously, data on masses and radii of these planets become more and more precise, allowing us to constrain compositions even further. In this work we calculated isothermal three-layer models for several known exoplanets with mean densities in the regime of rocky planets. Using different equations of state for both core and mantle materials we compare the results with regards to core size and thickness of the mantle layers and give estimates on possible compositions of these planets.

4.1 Thursday, 24.Sept.15, 11:00 (Invited)

Study of liquid iron alloys under extreme conditions

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The major portion of the Earth's core is in the liquid state, accounting for 18% of the total planetary volume. Although mostly composed of iron, it contains impurities that lower its density and melting point with respect to pure Fe. It is therefore important to determine melting relations and melting temperature of iron alloys under extreme conditions to constrain thermal structure and dynamic of the Earth's core. Although, with the recent discovery of extra-solar planets, planets with similar structures and masses up to 10 times the mass of the Earth open new questions concerning properties of iron and iron alloys under extreme conditions (330-1500 GPa, 5000-10000 K), with potentially a large portion that is in the liquid state. Here we will present way to investigate iron and its alloys from conditions of Earth's to Super-Earth's cores.

We will present XRD and XANES experimental results on liquid iron alloys measured using the Laser-Heated Diamond Anvil Cell (LH-DAC) up to multi-megabar conditions, obtained respectively on ESRF beamlines ID27 and ID24. We will discuss how each light element affect the local structure and the phase diagram of pure iron.

4.2 Thursday, 24.Sept.15, 11:30

Conductivity of iron along its melting curve

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Upon melting, many metals exhibit an increase of both compressibility β_T and electrical resistivity ρ_{el} . Since the ionic order is crucial to bulk elastic properties and the scattering probability of conduction electrons, β_T and ρ_{el} depend on the ion-ion structure factor $S(k)$.

We show that to first order, this behaviour on melting can be attributed to the change of $S(k)$ in the thermodynamic limit $k \rightarrow 0$. Using an equation of state and previous results for ρ_{el} in the liquid, we are able to compute electrical and – by way of the Wiedemann-Franz law – also thermal conductivity of solid iron up to the pressure of the Earth's inner core.

4.3 Thursday, 24.Sept.15, 11:50

Candy Wrapper for the Earth's Inner Core: Bridging Mineral Physics and Seismological Observations

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Recent global expansion of seismic data motivated a number of seismological studies of the Earth's inner core that proposed the existence of increasingly complex structure and anisotropy. In the meantime, new hypotheses of dynamic mechanisms have been put forward to interpret seismological results. Here, the nature of hemispherical dichotomy and anisotropy is re-investigated by bridging the observations of PKP(bc-df) differential travel-times with the iron bcc/hcp elastic properties computed from first-principles methods. The Candy Wrapper velocity model introduced here accounts for a dynamic picture of the inner core (i.e., the eastward drift of material), where different iron crystal shapes can be stabilized at the two hemispheres. We show that seismological data are best explained by a rather complicated, mosaic-like, structure of the inner core, where well-separated patches of different iron crystals compose the anisotropic western hemispherical region, and a conglomerate of almost indistinguishable iron phases builds-up the weakly anisotropic eastern side.

4.4 Thursday, 24.Sept.15, 12:10

Explaining lateral differences in inner core structure

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Seismic measurements show an east/west dichotomy in the outer 100 km of Earth's solid inner. This dichotomy could be explained by differential inner core growth with faster iron solidification in the western and possibly even melting in the eastern hemisphere during the last 100 Myr (or so). Two alternative scenarios could lead to such a pattern. In the first scenario a special translational convection mode leads to solidification in one hemisphere and melting in the other. However, latent heat and light elements expelled at the growing inner core front would then drive a hemispherical convection pattern in the outer core which seems not consistent with magnetic field observations. In the second scenario the outer core dynamics is the master and the inner grows faster where it is cooled more efficiently. We have implemented this second approach into the numerical MHD-code MagIC by parametrizing inner core growth and linking it to the outer core convective dynamics. Simulation results show that the new approach has little effect on the magnetic field and flow dynamics in the bulk of the core. While significant lateral variations in inner core growth are possible on shorter time scales, they tend to average out on time scales larger than 10 kyr. More or less homogeneous inner core growth is still promoted when imposing an inhomogeneous heat flux pattern at the outer boundary. We conclude that inner core growth purely driven by the outer core dynamics cannot explain the observed seismic dichotomy.

5.1 Thursday, 24.Sept.15, 14:00 (Invited)

Equations of state of metals from X-ray diffraction data at static pressures above 5 Mbar

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The impact of high-pressure studies on fundamental physics and chemistry, and especially on the Earth and planetary sciences, has been enormous. While experiments in diamond anvil cells (DACs) at pressures of ~250 - 400 GPa are proven to be very difficult but possible, at higher static pressures any matter has not been investigated until very recently. We have developed a method of synthesis of balls and semi-balls (of 10 to 50 μm in diameter) made of nanodiamond (with individual nano-particles of linear dimensions below 30 nm) and used them as second-stage or indenter-type anvils in conventional DACs. In experiments on rhenium, osmium, gold, platinum, and tungsten we were able to generate pressures above 700 GPa and demonstrated crucial necessity of the ultra-high pressure measurements for accurate determination of the equation of state of materials at extreme conditions. Especial attention has been paid on studies of osmium. Metallic osmium (Os) is one of most exceptional elemental materials having at ambient pressure highest known density, and one of the highest cohesive energy and melting temperature. Osmium is also very incompressible, once even claimed to be less compressible than diamond. However, osmium have been studied so far only at relatively low pressures below 70 GPa, and it necessarily limited accuracy of determined bulk modulus and provoke controversy regarding existence of isostructural transition at about 25 GPa. We investigated osmium by means of X-ray powder diffraction at multimegabar pressures using conventional and double stage diamond anvil cells. The bulk modulus of Os is high (414(1) GPa) but lower than that of diamond. While molar volume of osmium monotonically decreases with pressure, we found anomalies in the behavior of unit cells parameters ratio c/a at ~155 GPa and at ~435 GPa. Such effects may be related to electronic topological transitions similar to reported recently by us in isostructural with osmium high-pressure iron phase. We found that upon compression to over 750 GPa osmium remains in hexagonal close packed structure.

5.2 Thursday, 24.Sept.15, 14:30

Neutron Science in the megabar regime

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Neutron science at extreme conditions has a long history and indeed the first dedicated high-pressure beamline was actually built on a neutron source at the Idaho Falls Research Reactor in 1967. However, from the late 1980's, neutrons were somewhat overshadowed the coupling of megabar diamond anvil cells (DACs) and synchrotrons beginning in the 1980's. Up to the present day, the light sources have continued to dominate high-pressure research.

However, a quiet revolution has happened in the world of neutrons. In 2008 a next-generation facility, the Spallation Neutron Source (SNS), began operations in Oak Ridge. The SNS neutron beams, generated from a liquid mercury target, currently have the highest instantaneous brightness of any neutron facility. Within a further 2 years an even brighter neutron source, the Materials and Life Science Facility in Japan, came into operation. Most recently, in Sweden, 2014 saw construction begin at the European Spallation Source, which promises a further two orders of magnitude brightness increase on existing facilities when operational in 2019.

In parallel to these dramatic developments in neutronics, there have been concerted efforts to develop specialised DACs for static neutron diffraction measurements. These have successfully reached ~100 GPa at the SNS and will soon exceed this. This technology will mature rapidly as many of the technological challenges can be adapted, with minor modification, from synchrotron solutions. The current state-of-the-art in high-pressure neutron DAC work will be described along with some predictions for future capabilities.

5.3 Thursday, 24.Sept.15, 14:50

Free energy model for the high pressure solid phases of carbon

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Carbon plays an important role for the chemistry and physics of planets. In Neptune and Uranus for example the abundance of carbon in the form of methane amounts to 10-15% of the total mass. Methane can dissociate under the extreme conditions in the interior of these planets and may precipitate in the form of diamond [1].

It was suggested that carbon can also be a major constituent in extrasolar planets like the super-Earth 55 cancri e, which has been discussed to contain 10-70% of carbon [2] in the diamond phase.

The modeling of the interior structure of such planets requires precise knowledge of the phase diagram and equation of state (EOS) of carbon for a wide range of pressures and temperatures. A variety of high pressure phases has been proposed, including a body centered cubic phase with eight atoms in the unit cell (BC8) above 1 TPa, followed by a simple cubic (SC) phase above 2.9 TPa [3]. Both phases have yet to be confirmed experimentally.

In our work, we calculate a free energy model [4] for the diamond, BC8 and SC phases using the Vienna Ab Initio Simulation Package (VASP [5]), which is based on molecular dynamics for the ions and density functional theory for the electrons. This allows us to include anharmonic effects in the EOS. We investigate the diamond-BC8 and BC8-SC coexistence lines for temperatures up to 8000 K and compare with other theoretical predictions [6,7]. We also apply a thermodynamically constrained correction [8] to the EOS which brings our data in line with experimental results for low pressures.

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5.4 Thursday, 24.Sept.15, 15:10

Construction of a thermodynamic potential for the water ices VII and X

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Knowledge of the thermodynamic properties of the water ices VII and X is of significant importance for the interior modelling of water-rich giant planets and icy moons. We employ a combination of density functional theory (DFT), molecular dynamics (MD), and a variety of advanced postprocessing methods to construct an analytic thermodynamic potential (free energy) for ices VII and X [1]. In particular, the temperature-dependent part of the free energy function is constructed using entropy data obtained via the spectrum of vibrational modes from the MD simulations. Conceptual challenges due to the partial absence of stable zero-temperature states and proton disorder are overcome by performing calculations of representative crystalline states combined with a three-stage fitting procedure of data from MD simulations and static DFT calculations. The influence of the exchange-correlation functional is extensively discussed. Comparison with available experiments is made as well, and good agreement is achieved.

This work is supported by the Deutsche Forschungsgemeinschaft (DFG) within SFB 652 and SPP 1488.

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6.1 Friday, 25.Sept.15, 9:00 (**Invited**)

Mantle Rheology: Exploring Laboratory and Geophysical Constraints

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The rheology of the mantle plays a major role in mantle convection, plate motion, the path and fate of slabs, glacial isostatic adjustment, and large-scale tectonics. The rheological properties of the mantle have the first-order influence on questions regarding the mixing of materials within the mantle, the thermal evolution of the mantle. An understanding of the origin and evolution of the Earth requires an understanding of the rheological properties of the Earth's mantle.

There are three approaches to constraining mantle rheology: experimental studies of creep parameters; comparison of viscous flow models with geophysical observations, and guessing. There is a long and rich history of the latter. Due to the uncertainties of extrapolating from laboratory to geologic conditions, largely the large extrapolation in stress, experimental studies provide constraints on changes in viscosity as a function of temperature and grain-size. Geophysical constraints provide constraints on viscosity integrated over a finite depth interval and are thus non-unique. Rheology measurements are fit to an Arrhenius law. In the Arrhenius law the effect of pressure on viscosity is controlled by an activation volume and the effect of temperature on viscosity is controlled by the activation energy. The experimental constraints on the effect of pressure have large uncertainties and allow for either an increase or decrease in viscosity with depth. Because the Earth's temperature varies with depth, as expressed by the geotherm, the activation energy also has an indirect but significant effect on the radial profile of mantle viscosity. Furthermore, uncertainties in the distribution of water and grain-sizes throughout the mantle allow for a wide range of viscosity models.

6.2 Friday, 25.Sept.15, 9:30

Strength of (Mg,Fe)O ferropericlasite at high-pressures and high-temperatures and slab stagnation in the shallow lower mantle

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The Earth's lower mantle constitutes more than 50% of Earth's volume and is the largest geochemical reservoir for many elements. Material transport from Earth's surface into the deep mantle occurs by subduction of oceanic lithosphere. Seismic observations indicate stagnation and broadening of subducting slabs in the shallow lower mantle, but the underlying principle is unclear.

Ferropericlasite (Mg,Fe)O is thought to be the second most abundant mineral in Earth's lower mantle. Due to its potentially weak rheological behavior it may play a key role in controlling rheology, particularly in high strain areas in the Earth's mantle such as around subducting slabs.

Here, we present new results from synchrotron radial x-ray diffraction measurements on the deformation behavior of (Mg,Fe)O at high-pressures and high-temperatures. One set of experiments was performed on (Mg_{0.8}Fe_{0.2})O at the Advanced Light Source (Lawrence Berkeley National Laboratory) up to 96 GPa at 300 K. A second suite of data was collected at the Extreme Conditions Beamline of PETRA III (DESY) to 70 GPa at 850 K and 40 GPa at 1150 K.

From our data, we calculate the flow strength of ferropericlasite, which we find to increase by a factor of 3 at pressures from 20 to 65 GPa at 300 K. Modelling based on our experimental data indicates a 2.3 orders of magnitude increase of viscosity around subducting slabs in the upper 900 km of the lower mantle [1]. Such a strong viscosity increase can lead to stagnation of sinking slabs in the shallow lower mantle as observed by seismic tomography.

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6.3 Friday, 25.Sept.15, 9:50

High pressure phase diagram of MgO and FeO

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The state of matter (e.g. temperatures and pressures) inside super-Earths, i.e., planets in the mass range 1-10 M_E , 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 initio* 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 still under development but first results lead to good agreement with experimental results for the anti-ferromagnetic system of the B1 phase. Using the quasi-harmonic approximation the EOS is calculated and compared against available experimental data [8].

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6.4 25.Sept.15, 10:10

Fate of silicate melts at core-mantle boundary conditions

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The early vision of the mantle crystallizing from the bottom upwards towards the surface has been disputed due to computational data on melt densities supporting crystallization at an intermediate depth and an accumulation of dense melts in the deep mantle. The controversy between the two models arises because the exact nature of the partitioning of iron between solid and liquid phases in the lower mantle remains unclear. In addition, no experimental studies have measured directly the density of melts at the conditions of the deep mantle, even though it is the key parameter controlling the entrainment and/or settling of matter in the deep mantle.

Using a novel approach, we measured the density of MgSiO₃ amorphous glass in the small sample environment of the diamond anvil cell up to the core-mantle boundary pressure. We discovered that MgSiO₃ glass (300 K) and melt (4000 K) are as dense, within the uncertainties, as their crystalline MgSiO₃ Bridgmanite counterpart phases in the lowermost mantle. Our data on MgSiO₃ glass and melt provide the first experimental evidence for such high-density melts in the deep mantle.

Taking into account that iron will partition into the melt phase, we conclude that melting in the MgSiO₃-FeSiO₃ system will produce magmas that are denser than the residual solids, regardless of the exact nature of iron partitioning. This study therefore supports the theory of a deep basal magma ocean concomitant with the late accretion stage of the Earth. Such a magma ocean surrounding the core would be an ideal candidate for storing incompatible elements, thermally insulating the iron-rich core, thus delaying the crystallization time of the inner core.

7.1 Friday, 25.Sept.15, 11:00 (**Invited**)

Early thermomechanical evolution of planetesimals

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Here, we use 2-D and 3-D finite difference numerical models to study the early thermomechanical evolution of planetesimals and focus on the acapulcoite-lodranite meteorites, members of the primitive achondrite class. The observation of partial melting and resulting partial removal of Fe-FeS indicates that this meteorite group could be an important link between achondrite and iron meteorites, on the one hand, and chondrite meteorites, on the other. Thus, a better understanding of the thermomechanical evolution of the parent body of this meteorite group can help improve our understanding of the evolution of early planetesimals. By applying available geochronological, thermal, and textural constraints to our numerical data, we determine the formation time, initial radius of the parent body of the acapulcoite-lodranite meteorites, and their formation depth inside the body. Our data suggest that initial porosity has only a minor effect on the evolution of the parent body and that other meteorite classes could form at different depths inside the same parent body, supporting recently proposed models.

7.2 Friday, 25.Sept.15, 11:30

HIGH P-T DIFFUSION EXPERIMENTS IN LIQUID IRON

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Diffusive transport properties of molten iron and iron alloys at high pressures and temperatures are important for understanding planetary-scale processes, such as the physical and chemical differentiation of early-formed planetary interiors into silicate mantle and Fe-Ni alloy core reservoirs and their respective compositions, as well as the origin and evolution of geomagnetism, which is generally considered due to thermal and chemical convection in the liquid outer core. The density of the Earth's outer core is ~10-15% too low to be composed of pure Fe-Ni and is assumed to contain significant concentrations of light elements, such as Si and/or O, in addition to Cr, a siderophile transition metal that is depleted in the Earth's mantle relative to chondrites. In order to determine the pressure and temperature dependence of Si, O, and Cr chemical diffusion in molten iron, we have performed diffusion experiments between 3–18 GPa and 1915–2423 K using a multi-anvil apparatus.

High pressure laboratory diffusion couple experiments on low viscosity liquids are particularly challenging due to rapid equilibration of small (mm size) samples and non-isothermal annealing (i.e. diffusion during heating and quenching). The latter can result in an overestimation of the derived diffusion coefficients if the quenched diffusion profile is assumed to have formed solely at the peak annealing temperature. We solve the problem of non-isothermal heating numerically and refine diffusion parameters (i.e. activation energy and pre-exponential diffusion coefficient) using a finite difference least-squares fit solution to multiple (4-10) different diffusion profiles obtained at a given pressure but different temperatures, simultaneously. Our results show a very small pressure dependence ($< 1 \text{ cm}^3/\text{mol}$) of alloying element diffusion (Si, O, Cr) in liquid iron over the P-T range of the study and a remarkably good consistency with first principles calculations (Pozzo et al. 2013. Phys. Rev. B 87, 014110; Ichikawa and Tsuchiya. 2015. Phys. Earth Planet. Inter., in press) when extrapolated to outer core conditions.

7.3 Friday, 25.Sept.15, 11:50

Depth-dependence of viscosity and its influence on the Martian mantle dynamics

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The crustal dichotomy of Mars and volcanic landforms concentrated at a few volcanic provinces like Tharsis and Elysium have been interpreted as surface expression of a low degree mantle convection pattern in the interior of the planet [e.g. 1, 2]. The upcoming InSight (Interior exploration using Seismic Investigations, Geodesy and Heat Transport) mission, to be launched in 2016, will carry the first in-situ Martian heat flow measurement and provide an important baseline to constrain the present-day heat budget of the planet and, in turn, the thermal and chemical evolution of its interior. Although present-day variations of the surface heat flow are expected to be mainly influenced by variations in the thickness and radiogenic heat content of the crust [3], a non-negligible contribution may come from mantle plumes [4] whose number and shape strongly depends on the mantle rheology and in particular on the depth-dependence of the viscosity.

We run thermal evolution models for Mars in 3D spherical geometry [5] and vary the depth dependence of the viscosity to obtain possible low degree convection patterns for Mars. Literature values for the activation volume vary between 2 and 20 cm³/mol for diffusion creep [6], while some studies employ a viscosity jump in the mid mantle to model the effect of a phase transition [7]. In our calculations, we use the crustal thickness variations from [8], a low conductivity compared to the mantle and enriched in radiogenic heat producing elements. Our results show that including compressibility effects, phase transitions and different core sizes, surface heat flow variations are mainly dominated by the crust contribution, unless the radial mantle viscosity increases by more than one order of magnitude. All simulations show that present-day surface heat flow variations due to mantle upwellings remain confined to limited surface regions. However, the depth dependence of the viscosity can play a significant role for the convection pattern in the interior, whose signal may be visible in global heat flow maps. Narrowing the rheological parameter range by running ab initio calculations and high pressure experiments could help to constrain the interior dynamics of Mars and in particular its surface heat flow distribution.

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7.4 Friday, 25.Sept.15, 12:10

The curious case of Ganymede's magnetic field

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Ganymede's intrinsic, present-day dipolar magnetic field ($B_{\text{dip}}=719$ nT), whose existence puzzled the scientific community, is believed to be generated in its iron-rich core [1]. Since the present-day heat flux out of the core is too low to allow for purely thermal convection as

suggested from thermal evolution models for small planetary bodies such as Ganymede, e.g., [2], the core dynamo is most likely the result of compositional convection occurring during core differentiation [3]. It is assumed that the core of Ganymede consists of Fe-FeS - a composition generally taken to be a good model for Earth-like planetary cores. The core freezing scenario depends on the sulfur concentration in Ganymede's core and is also peculiar in comparison to Earth's core. Experimental work has shown that the slope of the liquidus, dT/dP , of the Fe-FeS eutectic is negative for the pressure range of Ganymede's core, e.g., [4], [5], and not positive as for Earth's core. As a consequence, crystallization starts at the core-mantle boundary (CMB) in the case of Ganymede. If the core contains less sulfur than the eutectic concentration, a snow zone containing sinking, solid Fe-crystals grows from the CMB to the core center (Fe-snow regime). If the core is more sulfur-rich than the eutectic concentration, an inward-growing, solid FeS-layer forms at the CMB (FeS-layer regime). For the Fe-snow regime, the remelting of Fe-crystals below the snow zone initiates compositional convection in the deeper core [6]. The dynamo in the Fe-snow regime is therefore restricted to the time the snow zone needs to grow across the core. In the FeS-layer regime, the growth of the FeS-layer induces an iron-rich liquid that is expelled at the freezing front. The dense iron-rich liquid is gravitationally unstable and compositional convection underneath the growing FeS-layer results in dynamo action in a similar manner as in the Fe-snow regime.

We ran a large set of Monte Carlo simulations based on parametrized thermal evolution models for Ganymede's mantle and core, spanning a wide range of parameters. We vary the initial amount of sulfur in the core, the initial temperature distribution, the reference viscosity of the mantle, the heat source density in the mantle, and the enrichment factor of radiogenic elements in the primordial crust. We investigate whether models exist that allow for a present-day dynamo in either the Fe-snow or the FeS-layer regime. We find that only 5% of all models can account for a present-day magnetic field. For successful models, we further find a relation between the initial sulfur concentration and the reference viscosity of the mantle. However, our study also suggests that apart from these two parameters the remaining input parameters remain unconstrained. Furthermore, in the case of the Fe-snow regime, the dynamo is a recent feature (less than ~ 1100 Myr old), whereas for the FeS-layer regime the dynamo can be as old as ~ 3100 Myr. In summary, our study shows that Ganymede's present-day magnetic field can be generated in a Fe-FeS core, but seems to remain a happenstance.

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P1 Wednesday, 23.Sept.15, 17:30

An upcoming facility for experimental studies of high-energy density states of matter: the HED science instrument at the European XFEL

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Free-electron laser facilities enable new applications in the field of high-pressure research including geo- and planetary sciences. At the European X-ray Free Electron Laser (XFEL) in Hamburg, one of the six baseline instruments is dedicated to High Energy Density Science (HED) [1]. The Helmholtz International Beamline for Extreme Fields (HIBEF [2]), which was approved earlier this year, will bring key-instrumentation to the beamline. The HED instrument is currently in its detailed design phase and first user operation is foreseen for late 2017.

At the HED science instrument, pump-probe experiments will be possible with a large choice of excitation sources including the FEL beam itself (delays of up to 2 -23 ps for 5 -20 keV using a split-and-delay unit), three optical lasers (either 200 kHz/3 mJ/15 fs, 10 Hz/100 TW/30 fs or 10 Hz/100J/ns), diamond anvil cells (laser-heated or dynamic) and pulsed magnetic fields (up to 50 T). Pump-probe experiments can be performed at adapted repetition rates (4.5 MHz, 1 – 10 Hz, shot on demand).

HED is located at the SASE2 undulator, which provides up to 27000 pulses per second with about 1012 photons per pulse, photon energies between 3 and 24 keV and pulse lengths of 2 – 100 fs to probe the samples at extreme states. Self-seeding is foreseen, as well as natural and wide SASE radiation. In addition, energy bandwidth of 10⁻⁴ and 10⁻⁶ will be made available through monochromators. Focussing is based on compound refractive lenses, which will allow to provide beam sizes in the sub-micrometer regime, 2 μm, 10-20 μm and 150 – 260 μm at the sample position. Available X-ray techniques comprise diffraction (XRD, SAXS), imaging (XI, PCI) and spectroscopic methods (XRTS, XANES, XES). The envisaged instrument time resolution is in the range of a few 10s fs.

In this contribution, we will show the current outline of the instrument and focus on experiments using the 100 J-class optical laser as a source. With its nanosecond pulse duration and the pulse shaping capability, it will allow to shock compressing matter to very high internal pressures of up to 1 TPa and to off-Hugoniot states at lower pressures with ramped compression [3] and thus allow studies of interiors of planets and exo-planets.

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P2 Wednesday, 23.Sept.15, 17:30

The HIBEF User Consortium

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The Helmholtz International Beamline for Extreme Fields (HIBEF) is a user consortium (UC) which contributes to the High Energy Density (HED) instrument of the European xFEL in Hamburg Germany. This includes different experimental setup and instrumentation, personal for installation and operation as well as building. In the center of interest are hereby plasma physics, high pressure science and high magnetic fields. Therefore the UC will provide one ultra-high intensity laser system and also a high-energy laser called DIPOLE. Additionally a complete setup for x-ray diffraction experiments under pulsed magnetic field up to 60 T is foreseen as well as a dedicated chamber for high pressure experiments using DACs respectively the high-energy laser for shock compression. The integration of all the devices contributed by the UC into the control system of HED will be done by the Helmholtz-Zentrum Dresden – Rossendorf (HZDR). Software tools for experiment simulation and data treatment will be provided.

Different Research Institutes and Universities all over the world evinced their strong interest in this UC. A proposal for funding of ~21 Mio€ was approved by the senate of the Helmholtz-Gemeinschaft in summer this years. Proposers are DESY (Deutsches Elektronensynchrotron Hamburg) and HZDR, which is also the leading institute. Additionally HIBEF-UK, lead by J. Wark, University Oxford, will provide the DIPOLE laser, constructed by the CLF and funded by STFC and EPSRC. HIBEF started the planning and design phase this year.

P3 Wednesday, 23.Sept.15, 17:30

Non-resonant Frequency-domain Interferometry for Probing the Phase Transitions of Silicon

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The study of reflectivity of a solid material during its irradiation, as well as the ultrafast dynamics associated with the relaxation of the system, has been the subject of numerous theoretical and experimental works in the past. Among the many techniques that have been developed over these years, Frequency-domain interferometry (FDI) can provide both time- and space-resolved measurements with high resolution¹⁻³.

In the present work, polarisation resolved FDI has been performed on a silicon target in order to determine the amplitude and the phase of the complex reflection coefficients to probe phase transitions (amorphization and fusion) induced by ultra-short laser pulses⁴. A part (70%) of the Aurore laser beam (1 kHz, 25 fs, 800 nm) was focused on the Si target (1 mm thick, <100> single crystal wafer) to trigger the phase transition. The remaining part of the beam (30%) was frequency converted through a non-collinear optical parametric amplifier (NOPA), finally delivering a 100 fs, 20 μ J probe pulse at 532 nm. Non-resonant pump-probe experiment has been therefore performed at different delays, up to 9 ps, and at different excitation levels, ranging from 50 to 350 mJ/cm². Post-irradiation analysis using optical microscopy, AFM and micro-Raman spectroscopy reveal three different materials modification thresholds, leading to amorphization or ablation. The threshold values for which the phase transitions of silicon was taking place were determined beforehand in order to perform the FDI measurements above each different threshold. The experimental results, currently under investigations, will be presented and discussed in terms of thermal and non-thermal processes with respect to recent theoretical results⁵.

This first demonstration of non-resonant, polarization-resolved FDI measurements pave the way to new insight in ultra-short structural dynamics of irradiated materials.

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P4 Wednesday, 23.Sept.15, 17:30

Time-resolved studies of phase transition dynamics

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The dynamics of pressure-induced phase transitions are leading to new discoveries and strategies for increased control of material microstructure, and by extension constitutive properties. Time-resolved x-ray scattering measurements of transitions provide unique microscopic insights into the dynamics of pressure-induced phase transitions; including nucleation, growth and the observations of intermediate and/or metastable phases. In addition, tunability of the pressure drive permits evaluations of the influence of compression rate. In this presentation we will discuss our studies of the dynamics of phase transitions under various compression rates in simple metals.

Portions of this work were performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and funded by the LLNL LDRD program under project tracking code 11-ERD-046. Portions of this research were carried out at Petra-III at DESY, a member of the Helmholtz Association (HGF). We thank the experimental support team lead by H.-P. Liermann for assistance in using the Extreme Conditions Beamline (ECB) P02.2. Portions of this work were performed at HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA under Award No. DENA0001974 with partial instrumentation funding by NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

P5 Wednesday, 23.Sept.15, 17:30

Thermal conductivity measurements in metals at high pressure and temperatures

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The transport properties of iron and iron alloys at high pressures and temperatures are crucial parameters in planetary evolution models, yet are difficult to determine both theoretically and experimentally. Estimates of thermal conductivity in the Earth's core range from 30 to 150 W/mK, a substantial range leaving many open questions regarding the age of the inner core, the thermal structure of the outer core, and the conditions for a working geodynamo. Most experiments have measured electrical resistivity rather than directly measuring thermal conductivity, and have used models to extrapolate to from low-temperature data to the high temperature conditions of the core. We present direct, in-situ high-pressure and high-temperature measurements of the thermal conductivity of metals in the diamond-anvil cell. Double-sided continuous laser heating is combined with one-side flash heating of a metallic foil, while the time-resolved temperature is measured from both sides with spectral radiometry in an optical streak camera. Emission and temperature perturbations measured on opposite sides of the foil were modeled using finite element calculations in order to extract thermal conductivity of foils. Results on platinum and iron at high pressures and temperatures will be presented.

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Keywords: Thermal conductivity, metals, Earth core, pulse laser heating

P6 Wednesday, 23.Sept.15, 17:30

Conceptual Design of the DAC setup for dsDAC and dDAC experiments at the HED instrument of the European XFEL

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Time resolved diffraction at simultaneous high-pressure and –temperatures as well as fast compression/heating is an emerging field in static/dynamic high-pressure physics. This technique may be used to determine Equation of State (EOS) and phase stability at very high pressures and temperatures using the double stage Diamond Anvil Cell (dsDAC, Dubrovinsky 2015) and the dynamic Diamond Anvil Cell (dDAC), which is not achievable with conventional static high-pressure techniques. In addition one may explore the effects of changing compression rates on the location and kinetics of solid-solid and solid-liquid phase transitions using the dynamic Diamond Anvil Cell (dDAC). While dynamic compression diffraction experiments are possible at 3rd generation sources in the kHz (ms) regime , it will require new 4th generation sources, such as the European XFEL, to be able to conducted time resolved experiments in the MHz (ns) regime.

In July of 2015 the Helmholtz Association decided to fund part of the “Helmholtz International Beamline for Extreme Fields” consortium headed by HZDR and DESY. Part of the project provides funding for a dedicated DAC setup to be installed at the High-Energy Density (HED) Instrument of the European XFEL. Within this presentation we describe the current status of the conceptual design for a dedicated DAC setup to conduct time resolved dynamic compression experiments in the dsDAC and dDAC.

P7 Wednesday, 23.Sept.15, 17:30

Novel LVP Techniques

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For extreme conditions experiments in Earth's and planetary materials research large volume presses (LVPs) and diamond anvil cells (DACs) are the suitable tools. DACs can reach Earth's core pressures and more. Classical LVPs are limited to a depth equivalent of about 1000 km, but the sample volume is 10^3 to 10^7 bigger and could be even further increased in principle. Latest since ultradeep subduction was verified by global seismic tomography we have to realize the existence of deep mantle complex rocks not less complex than metamorphic rocks known from Earth's surface sampling. The challenge is the physical properties of a complex system cannot be determined in principle if the volume under investigation is much smaller than the smallest component of the natural system under study. We also have to take into account that the physical properties of a complex system do not correspond to the sum of the properties of its constituents. The paper describes some novel approaches in extreme conditions research including the corresponding techniques for measuring the physical properties under in situ conditions.

P8 Wednesday, 23.Sept.15, 17:30

Properties of metastable high-pressure polymorphs of manganese oxides

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Technological needs require creating novel materials, and newly fabricated materials with advanced properties, in turn, lead to emergent industrial applications. In this work using a high-pressure high-temperature synthesis technique using multi-anvil assemblies we prepared and examined physical properties of high-pressure polymorphs of manganese oxides, including the perovskite-type ζ -Mn₂O₃ [1] and marokite-type γ -Mn₃O₄ [2]. These both polymorphs are readily recoverable at ambient conditions. The γ -Mn₃O₄ polymorph crystallizes in the CaMn₂O₃ (marokite)-type structure [2]. A recently discovered ζ -Mn₂O₃ with a triclinically-distorted double-perovskite-type structure has a very intricate electronic configuration, Mn²⁺(Mn³⁺)₃(Mn^{3.25+})₄O₁₂ [1]. We examined the optical and electronic transport properties of these polymorphs at ambient and high pressure. We found, in particular, that they both are narrow-band gap semiconductors, unlike the conventional wide-band-gap polymorphs of these oxide, cubic-bixbyite α -Mn₂O₃ and hausmannite α -Mn₃O₄. We investigated also the mechanical properties of these polymorphs using both nanoindentation and X-ray diffraction studies under high pressure. We compare the properties of these metastable manganese oxides with those of traditional non-oxide semiconductors.

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P9 Wednesday, 23.Sept.15, 17:30

High-pressure high-temperature synthesis of bulk $\text{Si}_{1-x}\text{B}_x$ alloys: two semiconductors form an unusual metal

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Silicon is a key technological material, and its controlled doping is one of simple and effective ways which are applied for creation of new advanced materials with tunable optoelectronic properties. Boron was known to be a dopant that can dramatically change the properties of silicon. However, a limited solubility of boron atoms in silicon matrix strongly restricted creation of bulk diamond-type structured Si-B alloys with the high boron content exceeding 0.5-1 at. %. In this work we used a high-pressure high-temperature synthesis technique to prepare bulk $\text{Si}_{1-x}\text{B}_x$ alloys. To generate high pressures we used both Piston-Cylinder apparatuses and Multi-Anvil Presses. The samples of Si:B were prepared from silicon and β -boron crystals. We found that alloying of boron and silicon can be strongly enhanced at high temperatures above the melting point of silicon and high pressures. We could synthesize the bulk $\text{Si}_{1-x}\text{B}_x$ alloys with a rather high boron content (e.g., 2.4 at.%).¹

We extensively investigated the electronic transport and optical properties of these alloys using several techniques, including electrical resistivity, Hall effect, magnetoresistance, Raman, infrared and optical spectroscopy, and X-ray diffraction. We found that $\text{Si}_{1-x}\text{B}_x$ solid solutions are metals that possess very unusual optical properties, e.g., they demonstrate the antiresonant Raman spectra and the loss of the reflectivity in the near-infra-red range. Our work indicates new perspectives in creation and applications of $\text{Si}_{1-x}\text{B}_x$ solid solutions with the diamond-type structure. This approach may be applied for doping of silicon and other materials with other dopants as well.

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P10 Wednesday, 23.Sept.15, 17:30

Investigation of the Magnesium Oxide phase diagram

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Understanding planetary interiors requires a detailed knowledge of the phase diagrams of planetary constituents. The abundance of MgO in the Earth's mantle and in exoplanet interiors makes it a good candidate for experimental and theoretical investigations. Indeed recently the phase diagram of MgO has been experimentally investigated with different techniques. In particular a recent decaying shock experiment proposed that MgO undergoes to a B1-B2 solid-solid phase transition at around 0.44 TPa and that it melts at 0.66 TPa [McWilliams]. A more recent laser-shock compression experiment seems to confirm the melting position but pushes the B1-B2 transition at lower pressure [Miyanishi]. At the same time, ab-initio calculations present contradictory results and incongruences with the experimental interpretation of the phase diagram [Cebulla, Boats and Bonev].

In this poster, we present the results of an experiment conducted at LULI 2000. Using the decaying shock technique, we investigated the phase diagram of MgO measuring shock velocity, temperature and reflectivity at two wavelengths along the Hugoniot in the pressure range 0.25 - 1.4 TPa. Our shots were executed varying laser parameters and ablator materials to change the hydrodynamics on the decaying shock. We present the data analysis, showing some differences with previous experiments. A preliminary interpretation is presented.

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P11 Wednesday, 23.Sept.15, 17:30

Calculations of phonon spectra from ab-initio MD simulation

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CEA Arpajon

In density functional theory the thermal vibration of atoms and therefore the free energy are usually obtained via the harmonic or quasiharmonic approximation. Unfortunately, it is well known that this approximation fails for the treatment of lattice dynamics of strongly anharmonic solids. For example, the free energy of dynamically unstable structure at 0 K as the bcc structure of Li, Zr, Ti or U cannot be obtained or the temperature dependence of a soft mode cannot be reproduced. Here we will present how the lattice dynamics of a solid at high temperature can be obtained by means of first-principles molecular dynamics simulations[1]. Then we will present several examples to show the usefulness of this method: the B1-B2 phase transition in MgO and the sound speeds of pure iron.

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P12 Wednesday, 23.Sept.15, 17:30

Mercury's thermal evolution and core crystallisation regime

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Unlike the Earth, where the liquid core isentrope is shallower than the core liquidus, at the lower pressures inside Mercury's core the isentrope can be steeper than the melting temperature. As a consequence, upon cooling, the isentrope may first enter a solid stability field near the core mantle boundary and produce iron-rich snow that sinks under gravity and produces buoyant upwellings of iron depleted fluid. Similar to bottom up crystallization, crystallization initiated near the top might generate sufficient buoyancy flux to drive magnetic field generation by compositional convection.

In this study we model Mercury's thermal evolution by taking into account the formation of iron-rich snow to assess when the conditions for an internally magnetic field can be satisfied. We employ a thermodynamic consistent description of the iron high-pressure phase diagram and thermoelastic properties of iron alloys as well as the most recent data about the thermal conductivity of core materials.

P13 Wednesday, 23.Sept.15, 17:30

Geodynamics of Mercury: MESSENGER spacecraft observations, equation of state, and rheology constraints

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Of all the rocky planets in our solar system, the innermost planet, Mercury, has long been known to have the largest iron core relative to the planet radius. Gravity and shape data from the MESSENGER spacecraft place even tighter constraints on the size of Mercury's core and the density of Mercury's silicate outer shell [1]. These observations require that the silicate mantle is even thinner than previously assumed, which suggest that solid-state convection in Mercury's silicate mantle is, at best, marginally supercritical. At the same time, surface compositions inferred from MESSENGER data are consistent with lavas that formed from high-temperature and/or high-degree of partial melts of the mantle [2]. The high temperature magmas and observations of tectonic deformation indicate that the mantle was actively deforming much later in Mercury's evolution than previous models predicted [3]. These apparently contradictory observations can be resolved by recognizing that at the low pressures of Mercury's silicate mantle, deformation is likely to be dominated by dislocation (power-law) creep rather than diffusion creep.

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P14 Wednesday, 23.Sept.15, 17:30

Crystallizing the Martian Magma Ocean

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The structure of terrestrial planets with a solid mantle may have evolved from a largely molten stage through fractional crystallization. If the solidification produced an unstable density stratification, the structure of the planet may have undergone further changes governed by the mechanics of mantle convection, possibly including a catastrophic overturn of the entire mantle. We explore a possible scenario for the crystallization of the Martian mantle from a magma ocean based on a combination of experimental major element partitioning data and thermodynamic modeling. From our model we compute geodynamically relevant parameters for the resulting layers of rock immediately after solidification, such as density profile, total radius of the planet and moment of inertia.

P15, Wednesday, 23.Sept.15, 17:30

Observability of shape distortion of exoplanets with future space observatories

Szilard Csizmadia

DLR Berlin

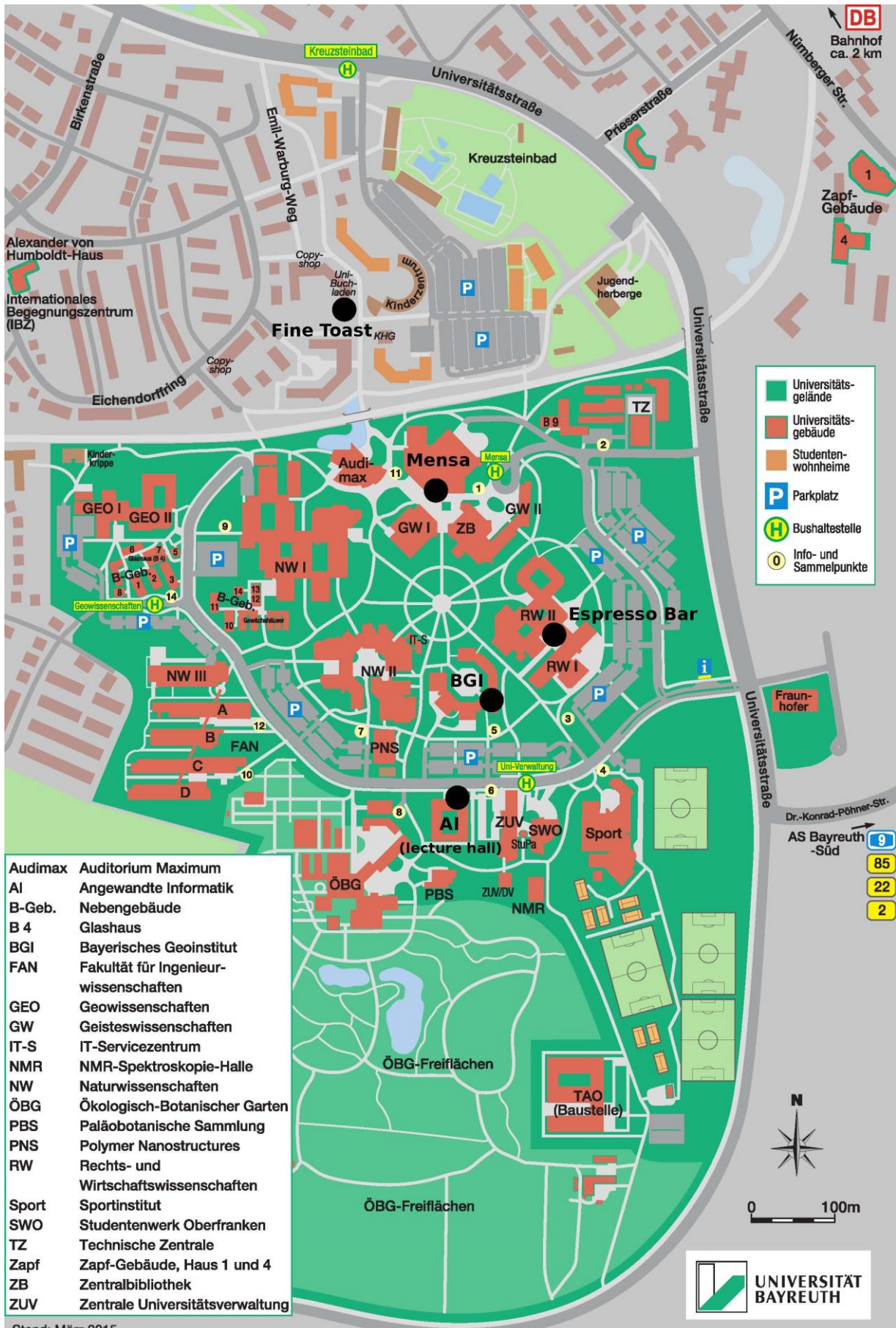
Nowadays we fit the exoplanet transit light curves with a spherical planet-model. But the shape of an exoplanet is related to the Love-number k_2 , its rotational period etc. therefore it would be important to establish the true shape of exoplanets. The transit light curve contains this kind of information. We present synthetic light curves to estimate the range of the effect what a distorted shape causes and we compare the light curves obtained by using a spherical planet model and a Roche-model. We point out that this effect would be observable with future space observatories and, in certain cases, in the presently available light curves, too. Then, this shape distortion could be related to the internal mass distribution of an exoplanet which is not known yet.

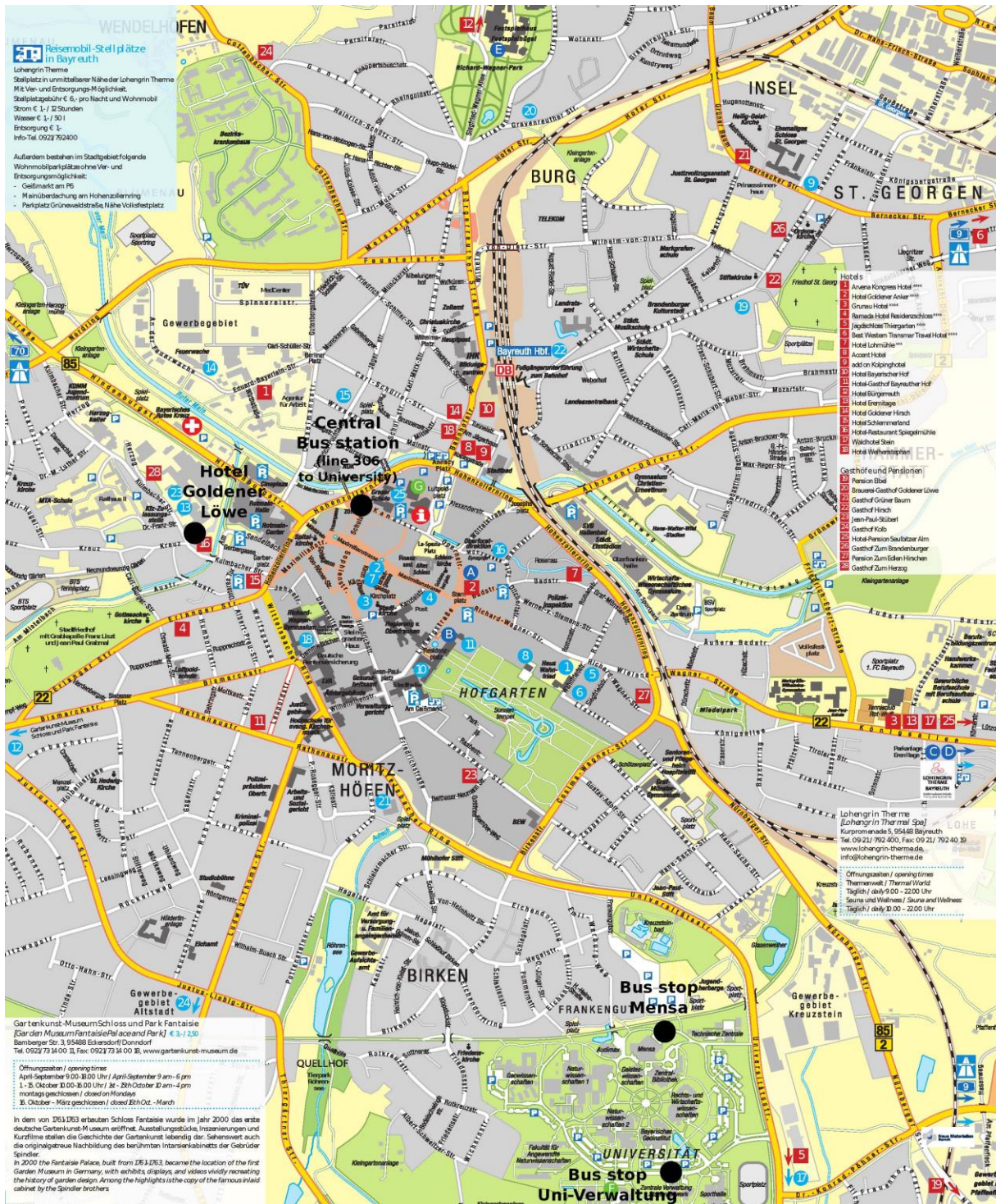
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Maps





4th Joint Workshop on High Pressure, Planetary and Plasma Physics (4HP4)					
Bayreuth, September 23-25, 2015					
Program short					
Wednesday, September 23		Thursday, September 24		Friday, September 25	
Arrival		9:00	Datchi	9:00	King
		9:30	Nettelmann	9:30	Marquardt
		9:50	Duarte	9:50	Cebulla
		10:10	Kellermann	10:10	Petitgirard
		10:30	Coffee break	10:30	Coffee break
		11:00	Morard	11:00	Golabek
		11:30	Wagle	11:30	Posner
12:00	Registration	11:50	Mattesini	11:50	Plesa
12:00	Light lunch	12:10	Wicht	12:10	Rückriemen
13:45	Opening	12:30	Lunch break	12:30	Conclusion
14:00	McWilliams	14:00	Dubrovinsky	Departure	
14:30	Gericke	14:30	Guthrie		
14:50	Bethkenhagen	14:50	Schöttler		
15:10	Zastrau	15:10	French		
15:30	Coffee break	15:30	Coffee break		
16:00	Monaco	16:00	Lab tours		
16:30	Appel				
16:50	Redmer				
17:10	Recoules				
17:30	Posters				
18:00	HIBEF Meeting	19:30	Conference dinner		



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