Joint Workshop on High Pressure, Planetary, and Plasma Physics

DLR Berlin-Adlershof
Institute of Planetary Research
October, 10th – 12th, 2018

Deutsches Zentrum
DLR für Luft- und Raumfahrt e.V.
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Joint Workshop on High Pressure, Planetary, and Plasma Physics

7th Joint Workshop on High Pressure, Planetary, and Plasma Physics
October 10 – 12, 2018
DLR, Institute of Planetary Research, Berlin, Rutherfordstraße 2
Meeting Room: Rotunde

The main objective of this workshop is to bring together scientists from different fields of expertise to discuss topics related to extreme planetary environments in terms of high temperature and high pressure. This meeting is also intended to inspire new projects and offer scientific opportunities for future collaboration between workshop participants from distinct research fields.

Meeting website for more information, registration, abstract submission, and logistical details:

https://indico.desy.de/indico/event/18893/

SOC: Doris Breuer, Hanns-Peter Liermann, Ronald Redmer, Tina Rückriemen-Bez, Frank Sohl, Gerd Steinle-Neumann, Thomas Tschentscher.

LOC: Renate Schubert, Mellina Hurryman, Doris Breuer, Tina Rückriemen-Bez, Frank Sohl.

Previous Workshops

1st HP4 DESY Hamburg 2012 (Science beyond 4 Mbar and using dynamic compression)
https://indico.desy.de/indico/event/6024/

2nd HP4 DLR Berlin 2013
https://indico.desy.de/indico/event/8221/

3rd HP4 University Rostock 2014
https://indico.desy.de/indico/event/9404/

4th HP4 BGI Bayreuth 2015
https://indico.desy.de/indico/event/12227/

5th HP4 DESY Hamburg 2016
https://indico.desy.de/indico/event/14266/

6th HP4 MPI Göttingen 2017
https://indico.desy.de/indico/event/16402/

7th Joint Workshop on High Pressure, Planetary, and Plasma Physics (HP4)
October 10-12, 2018

Conference Program

Wednesday, October 10		
12:00	Registration in DLR, Rutherfordstr. 2, 12489 Berlin	
13:30	Welcome and Introduction	**Rauer**
13:35	Chemical and isotopic constraints on the composition of the terrestrial planets *(Opening Talk)*	**Becker**
Session I: Interior and Atmospheres of Exoplanets Chair: Wicht		
14:20	*Remote Sensing of the Atmospheres of Exoplanets (Invited)*	**Heng** (p.11)
14:50	Modeling young Hot Jupiters as a window to formation processes - Do clouds influence the interior models of giant planets?	**Poser** (p.12)
15:10	Coffee Break	
15:40	Measurability of the fluid Love number k2 in WASP-121b	**Hellard** (p.13)
16:00	Matrix-propagator approach to compute fluid Love numbers and applicability to extrasolar planets	**Padovan** (p.14)
16:20	Effects of different equations of state on interior models of exoplanets	**Baumeister** (p.15)
16:40	Coffee Break	
Session II: Molecular Systems I Chair: French		
16:50	Diamond strength measurements above the Hugoniot elastic limit *(Invited)*	**Fletcher** (p.16)
17:20	Miscibility gap of hydrogen-helium mixtures	**Schöttler** (p.17)
17:40	Equation of state and optical properties of shock-compressed C:H:N:O mixtures	**Guarguaglini** (p.18)
18:00	Poster Session (Drinks and Snacks)	

Thursday, October 11

Session III: Rocky/Icy Planets and their Materials
Chair: Rivoldini

Time	Title	Speaker	Page
9:00	Iron and Iron alloys under extreme conditions for geoscience application	**Harmand**	(p.19)
9:20	On the trail of Uranus' and Neptune's diamonds via laboratory experiments using laser induced shock compression	**Schuster**	(p.20)
9:40	Ab initio study of Magnesium Oxide Properties under Super-Earth interior conditions	**Soubiran**	(p.21)
10:00	Structural studies of minerals and compounds at pressures above 200 GPa	**Khandarkaeva**	(p.22)
10:20	Mass-radius relations of rocky exoplanets and the B1-B2 mantle phase transition of ferropericlase (Mg,Fe)O	**Sohl**	(p.23)
10:40	Coffee Break		

Session IV: Rocky Planets and their Evolution
Chair: Plesa

Time	Title	Speaker	Page
11:10	Magma ocean crystallization and terrestrial planets dynamics	**Maurice**	(p.24)
11:30	Volatile degassing and chemical speciation of the C-O-H system in the Earth Magma Ocean scenario	**Ortenzi**	(p.25)
11:50	Stratification of Mercury's core	**Deproost**	(p.26)
12:10	Constraints on the lunar core composition and thermal state from geophysical data and thermodynamic properties of liquid iron-sulfur alloys	**Rivoldini**	(p.26)
12:30	Lunch Break		

Session V: DAC Techniques and Applications
Chair: Liermann

Time	Title	Speaker	Page
13:30	Simulating the effects of shock compression in dynamic diamond anvil cell experiments *(Invited)*	**Langenhorst**	(p.27)
14:00	The Dynamic Resistive-Heated Diamond Anvil Cell: Compression under controlled compression rates and high temperatures	**San Jose Mendez**	(p.28)
14:20	New design of double-stage diamond anvils shaped from single crystal diamond plate	**Dubrovinsky**	(p.29)
14:40	Toroidal diamond anvils for static compression experiments beyond 5 megabar	**Jenei**	(p.30)

15:00	Coffee Break		
Session VI: Gas Giants **Chair: Nettelmann**			
15:30	The interior of Jupiter *(Invited)*	**Helled**	(p.31)
16:00	The interior of Jupiter with Juno constraints: Importance of Equations of State	**Guillot**	(p.32)
16:20	Dynamo Action of Jupiter's Zonal Flows	**Wicht**	(p.33)
16:40	Discussion		
17:00	**End of Session**		
19:00	Conference Dinner at **Ratskeller Köpenick, Alt-Köpenick 21, 12555 Berlin** https://www.ratskeller-koepenick.de/en/		

Friday, October 12		
Session VII: XFEL and Shock Methods Chair: Tschentscher		
9:00	Measuring Plasma Parameters of Warm Dense Matter from X-Ray Thomson Scattering at the LCLS and the NIF *(Invited)*	**Witte** (p.34)
9:30	Rapid Target Heating with High Intensity XFEL Beams	**Hartley** (p.35)
9:50	Studies of matter at extreme conditions using hard X-ray FELs	**Appel** (p.36)
10:10	Polymorphism, amorphization and melting of SiO_2 and Mg-bearing silicates from in-situ X-ray diffraction of laser-driven shock-compression	**Hernandez** (p.37)
10:30	Coffee Break	
Session VIII: Molecular Systems II Chair: Husband		
11:00	Theory and simulations of the compressive freezing to ice VII *(Invited)*	**Belof** (p.38)
11:30	Proton dynamics in high-pressure ice-VII from density functional theory	**Trybel** (p.39)
11:50	Thermal conductivity of water plasmas from ab initio simulations	**French** (p.40)
12:10	Final Discussion	
12:30	**End of Workshop**	

List of Posters

Abdussalam	Electronic stopping power of warm dense matter from TDDFT - Ehrenfest dynamics	(p.41)
Belof	Nanosecond freezing of water near the metastability limit	(p.41)
Bender Koch	Do impactites contain metal condensate from evaporated meteorite?	(p.42)
Bethkenhagen	DFT+U equation of state for iron oxide	(p.43)
Csizmadia	Love-number of WASP-18Ab	(p.44)
Doherty	Multicomponent Melting in a Heterogeneous Lunar Mantle after Magma Ocean Solidification	(p.45)
Husband	Isotopic shift of the insulator-metal transition in dense fluid hydrogen	(p.46)
Liermann	Implementations of DAC setup for DACS, DSDAC and DDAC experiments at the HED instrument of the European XFEL	(p.47)
Nettelmann	Static Love number k_{nm} values of Jupiter from interior models	(p.48)
Otzen	DFT Calculations of the linear elasticity of quartz and implications for pressure-induced lamellar amorphization	(p.49)
Ovsyannikov	High-pressure behavior of Fe_4O_5 at low and high temperatures	(p.50)
Plesa	Seismic velocities in the martian mantle and crust calculated from a 3D thermal and mineralogical model	(p.51)
Plückthun	The dynamic diamond anvil cell (dDAC) at the HED instrument of the European XFEL	(p.52)
Preising	The Melting Line and the Band Gap of Helium	(p.53)
Ramakrishna	First-principles study of the electronic structure and dielectric response function of diamond and other relevant high pressure phases of carbon up to 15 Mbar	(p.54)
Redmer	Paramagnetic-to-diamagnetic transition in dense liquid iron and its influence on electronic transport properties	(p.55)
Ruedas	Synthetic geophysical observables from martian mantle convection models, with application to InSight	(p.56)
Rückriemen	The Martian dynamo powered by Fe snow	(p.57)
Scheibe	Towards a new tool for modelling non-adiabatic giant planets	(p.58)
Schölmerich	Structure of SiO_2 melts at ultrahigh pressures – the experimental and ab initio approach	(p.59)

Abstracts

Session I - Atmospheres and Interiors of Exoplanets

REMOTE SENSING OF THE ATMOSPHERES OF EXOPLANETS

Kevin HENG (University of Bern)

There is tremendous excitement for exoplanet science, which is beginning to experience an influx of talent and expertise from outside of astronomy and astrophysics. There is a list of 'grand challenges' in exoplanet science, but one remains central: the remote sensing of the atmospheres of exoplanets. It has become abundantly clear that questions regarding habitable worlds require a perspective beyond the Solar System, to respect but also ultimately discard our Earth-centric perspective. Short of mastering interstellar travel, remote sensing using spectroscopy of exoplanets is the only way to address questions beyond their radii, masses and bulk densities. Since surface and subsurface properties are not directly measurable, the atmosphere of an exoplanet provides a valuable window into its climate and formation history. In the current talk, I will discuss the challenges associated with solving this inverse problem of inferring the physical and chemical properties of an exoplanetary atmosphere from the observed transmission and emission spectra, known in exoplanet science as 'atmospheric retrieval'. Atmospheric retrieval is fraught with degeneracies. With transmission spectra of transiting exoplanets, this is the need to overcome the 'normalisation degeneracy', which states that there is an ambiguity between the absolute normalisation of the spectrum, the abundance of molecules and a reference pressure. With emission spectra of non-transiting objects (both exoplanets and brown dwarfs), the challenge is to correctly retrieve physically meaningful values for the radii and gravities. Furthermore, there is the explosive development of using ultra-high-resolution ground-based spectroscopy to directly identify atoms and molecules in exoplanetary atmospheres. I will mention our team's recent discovery of atomic iron and titanium in KELT-9b, which is the first time these elements have been observed directly in an exo-atmosphere. Several teams worldwide are commissioning these spectrographs, including ESPRESSO with an unprecedented spectral resolution of ~10 cm/s, which motivates a closer look at the underlying theory. I will discuss cutting-edge machine learning techniques used to interpret these spectra. In the final accounting, my perspective is that if it is neither derivable from first principles (either theory or experiment) nor falsifiable (being able to prove that a hypothesis is wrong) by the astronomical data, then the question is not worth asking.

MODELING YOUNG HOT JUPITERS AS A WINDOW TO FORMATION PROCESSES - DO CLOUDS INflUENCE THE INTERIOR MODELS OF GIANT PLANETS?

Anna Julia POSER (University of Rostock)

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Ronald REDMER (University of Rostock)

Giant planets are important astrophysical objects as they shape planetary systems. We aim at understanding their formation processes and evolution scenarios of planetary systems. Basic correlations such as that between the planetary heavy element mass and the stellar metallicity [1,2] are key in this context. We determine the core mass Mcore of the planet as a representative of the heavy element mass by the combination of atmosphere, structure, and evolution calculations. As transiting gaseous planets are strongly irradiated by their parent stars and transmission spectroscopy indicates the presence of clouds, we investigate the influence of different atmosphere models on the derived heavy element mass. We use atmospheric profiles with and without clouds based on a semi-analytical atmosphere model [3,4]. We find that the applied model atmosphere does not change the energy balance, nor does it influence the convective interior. In particular, low-opacity clouds in the upper atmosphere, i.e. P < 1 bar, have low influence on the predicted core mass. On the other hand, optically thick clouds in the lower atmosphere, i.e. P > 10 bar show strong influence on Mcore of about 30 – 50 ME for higher intrinsic temperatures Tint. In future work we will compare to different atmosphere models, such as HELIOS [5], and an improved treatment of opacities, i.e. using non-grey opacities.

References:
[1] Guillot et al. 2006, A&A 453:L21
[2] Thorngren et al. 2016, ApJ 831:64
[3] Guillot 2010, A&A 520:A27
[4] Heng et al. 2012, MNRAS 420:20
[5] Malik et al. 2017, AJ 153:2

MEASURABILITY OF THE FLUID LOVE NUMBER K_2 IN WASP-121B

Hugo HELLARD (DLR Berlin)

Szilard CSIZMADIA (DLR Berlin)
Heike RAUER (DLR Berlin, FU Berlin, TU Berlin)

We are witness to a great and increasing interest in internal structure, composition and evolution of exoplanets [1]. However, direct measurements of exoplanetary mass and radius are insufficient to distinguish between different internal structure and composition models [2]. Hence, we need an additional observable to further constrain the internal structure of exoplanets. Because of observational reasons, most of the detected exoplanets are close-in objects, with typical orbital periods less than ten days [3]. Such planets undergo strong tidal deformations coming from their host star, as well as rotational deformations, modifying their outer shape from spherical to more complicated ones. We assume that both components are in hydrostatic equilibrium, i.e. the shape is relaxed. This implies that the body responds instantaneously to any external perturbation, hence behaving as a fluid. The resulting surficial deformations depend on the internal structure of the planet, and may be expressed through the fluid Love numbers [4]. These numbers describe the component's response to any external perturbing potential, and solely depend on the internal radial density distribution [5]. In particular, the second degree fluid Love number k_2 expresses the mass concentration towards the component's center, hence providing additional information about the internal structure. We present a new model that computes transit light curves of exoplanets under tidal and rotational deformations, beyond the usual mass-point approximation (i.e. Roche model [6]). We discuss detectability and measurability of k_2 in the transit curves of the hot Jupiter WASP-121b in the light of previous and future space observatories (e.g. Kepler, TESS, JWST, PLATO) [7].

References:
[1] Schneider, (2017).
[2] Zeng et al., 2016; Hatzes & Rauer, 2015; Wagner et al., (2011).
[3] exoplanets.eu
[4] Love, (1911); Kopal, (1959).
[5] Kellermann et al., (2018); Love, (1911).
[6] Wilson & Devinney, (1979).
[7] This work is supported by the DFG within the FOR 2440 "Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics."

MATRIX-PROPAGATOR APPROACH TO COMPUTE FLUID LOVE NUMBERS AND APPLICABILITY TO EXTRASOLAR PLANETS

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The mass and radius of a planet directly provide its bulk density, which can be interpreted in terms of its overall composition. Any measure of the radial mass distribution provides a first step in constraining the interior structure. The fluid Love number k_2 provides such measure, and estimates of k_2 for extrasolar planets are expected to be available in the coming years thanks to improved observational facilities and the ever-extending temporal baseline of extrasolar planets observations. We describe a method based on the classical matrix propagator technique to easily calculate the fluid Love numbers k_n ($n >= 2$) starting from a discretized radial density profile. The code is fast, freely available, and easy to combine with preexisting interior structure codes. While this approach cannot treat the presence of nonlinear effects that may arise under certain dynamical conditions, it is applicable to close-in gaseous extrasolar planets like hot Jupiters, likely the first targets for which k_2 will be measured [1,2].

References:
[1] Padovan et al., submitted to A&A.
[2]This work is supported by the DFG within the FOR 2440 "Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics" (grant SO 349/2-1).

EFFECTS OF DIFFERENT EQUATIONS OF STATE ON INTERIOR MODELS OF EXOPLANETS

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One of the major aspects of current exoplanetary science is the characterization of the planetary interior. A common approach to characterize the interior of a known exoplanet is the use of numerical models to compute a radially-dependent density distribution which complies with the measured mass and radius of the planet [1,2]. In general, however, possible solutions are highly degenerate, with multiple, qualitatively different interior compositions that can match the observations equally well. In order not to increase further any intrinsic degeneracy, it is also important to assess the impact of different model parameterizations. In this work, we quantify the influence of different isothermal and temperature-dependent equations of state (EoS) usually employed for metallic cores and rocky mantles on the computation of the interior structure of exoplanets. We perform an extensive parameter study modelling a vast number of sub-Neptunian exoplanets of different bulk composition, ranging from super-Earths, consisting just of a metallic core and a silicate mantle, to sub-Neptunes, including ice and gaseous layers. We find that the choice of EoS for the mantle has little influence on the characterisation of the interior structure of the planet, whereas small changes in the mineralogical composition of the planetary layers can lead to double digit uncertainties [3].

References:
[1] Sotin et al. (2007).
[2] Seager et al. (2007).
[3] This work is supported by DFG through the Priority Program 1922 "Exploring the diversity of extrasolar planets" (grant TO 704/3-1).

Session II – Molecular Systems I

DIAMOND STRENGTH MEASUREMENTS ABOVE THE HUGONIOT ELASTIC LIMIT

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Shear strength provides a fundamental description of a material's mechanical behavior during dynamic compression and it plays an essential role in the absolute knowledge of the material's equation of state (EOS). Experiments were conducted at the Matter in Extreme Conditions (MEC) end-station of the Linac Coherent Light Source (LCLS) to laser shock compress polycrystalline diamond to pressures above 3 Mbar. In our study, 527-nm, 10-ns, 25-J laser beams were used to irradiate 25 μm thick mylar ablators thereby launching shockwaves into 40 μm thick polycrystalline diamond samples. The compressed samples were then probed using the LCLS, operating in self-amplified spontaneous emission (SASE) mode, to provide 2 mJ of 10 keV x-rays in 50 fs pulses with 50 eV full-width at half maximum spectral bandwidth (0.5%). We calculate dynamic material strength by combining direct lattice strain measurements from x-ray diffraction (XRD), wave profiles measurements from velocity interferometry (VISAR), and ab initio calculations of elastic constants using density functional theory (DFT). We determine the strength of shock-compressed polycrystalline diamond at stresses above the Hugoniot elastic limit using a novel technique combining x-ray diffraction with velocity interferometry. These measurements, in addition to calculated elastic constants, allow for the first comprehensive determination of material strength above the Hugoniot elastic limit.

MISCIBILITY GAP OF HYDROGEN-HELIUM MIXTURES

Manuel SCHÖTTLER (Universität Rostock)

Ronald REDMER (Universität Rostock)

We calculate the high-pressure demixing phase diagram of hydrogen-helium mixtures [1], which is important for applications in planetary physics, in particular, for calculating the interior and evolution of gas giants. The separation of hydrogen and helium has long been proposed as a possible source of Saturn's excess luminosity: The initially hot planet cools down with increasing age and when the planetary isentrope intersects with the demixing region [2], helium-rich droplets can form and sink toward the planetary core, thus, acting as an additional source of heat; see, e.g., [3]. The region of demixing is observed from thermodynamic relations by computing the free enthalpy G(x,P,T) at constant pressure P and temperature T for different helium fractions x. We use finite-temperature density functional theory molecular dynamic simulations to obtain the equation of state for given volumes and temperatures. The non-ideal entropy of mixing is calculated using a combination of coupling-constant integration and thermodynamic integration of the equation of state. The choice of an appropriate exchange-correlation (XC) functional is of paramount importance. It has been shown that standard approximations such as PBE lack the ability to adequately describe the metallization transition in hydrogen [4], which is directly connected to the H-He demixing. Functionals that take into account non-local correlations such as vdW-DF [5] are in better agreement with recent experiments [4]. Benchmarking studies with many XC functionals against QMC calculations suggest vdW-DF as an appropriate functional also for hydrogen-helium mixtures [6]. Here, we present a demixing phase diagram of H-He mixtures calculated with vdW-DF and compare with previous calculations derived with the PBE functional [7,8]. Differences and implications for planetary physics are discussed, in particular, for the gas giants Jupiter and Saturn.

References:
[1] Schöttler and Redmer, PRL 120, 115703 (2018).
[2] Stevenson, PRB 12, 3999 (1975).
[3] Püstow et al., Icarus 267, 323 (2016).
[4] Knudson et al., Science 348, 1455 (2015).
[5] Dion et al., PRL 92, 246401 (2004).
[6] Clay et al., PRB 89, 184106 (2014).
[7] Lorenzen et al., PRL 102, 115701 (2009).
[8] Morales et al., PRB 87, 174105 (2013).

EQUATION OF STATE AND OPTICAL PROPERTIES OF SHOCK-COMPRESSED C:H:N:O MIXTURES

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Water, ethanol, and ammonia are amongst the key components of Uranus and Neptune. Knowing their equation of state, conductivity, and transport properties at planetary interiors conditions (a few Mbar and a few 1000 K) is required for developing precise structure and evolution models of the two planets as well as for explaining their puzzling magnetic fields and luminosities. The physical and chemical behavior of such mixtures at extreme pressures and temperatures is not only important for planetology but also interesting on its own, since those conditions are characterized by the coexistence of dissociated atoms, atomic clusters and chains. This regime is very difficult to study via ab initio simulations and experimental verifications are required. We studied pure water, a C:H:O and a C:H:N:O mixture, compressed up to 2.8 Mbar via laser-driven shock loading. The principal Hugoniot has been explored using the decaying shock technique. Moreover, off-Hugoniot states have been reached via a double-shock technique and through coupling of dynamic and static compression in diamond anvil cells. The experiments were performed at the GEKKO XII and LULI 2000 laser facilities using standard rear-side optical diagnostics (VISARs, SOP, reflectometer) to characterize the equation of state (a relation between density, pressure, internal energy, and temperature) and optical reflectivity of the shocked state. The results show that water and C:H:N:O mixtures share the same equation of state with a trivial density scaling, while the reflectivity behaves differently in both the onset pressure and the saturation value. From the reflectivity measurements at two different frequencies an estimation of conductivity and of the refractive index will be given using a Drude model. The consequences for the icy giants' interiors will be addressed.

Session III – Rocky/Icy Planets and their Materials

IRON AND IRON ALLOYS UNDER EXTREME CONDITIONS FOR GEOSCIENCE APPLICATION

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An accurate knowledge of the properties of iron and iron alloys at high pressures and temperatures is crucial for understanding and modelling planetary interiors. While Earth- size and Super-Earth Exoplanets are being discovered in increasingly large numbers, access to detailed information on liquid properties, melting curves and even solid phases of iron and iron at the pressures and temperatures of their interiors is still strongly limited. In this context, XFEL sources coupled with high-energy lasers afford unique opportunities to measure microscopic structural properties at far extreme conditions. Also the achievable time resolution allows the shock history and phase transition mechanisms to be followed during laser compression, improving our understanding of the high pressure and high strain experiments. Here we present recent studies devoted to investigate the solid-solid and solid- liquid transition in laser-shocked iron and iron alloys (Fe-Si, Fe-C and Fe-O alloys) using X-ray diffraction, X-ray diffuse scattering and X-ray absorption spectroscopy. Experiments were performed at the MEC end-station of the LCLS facility at SLAC (USA) and at the EH5 end-station of the SACLA facility (Japan). Detection of the diffuse scattering allowed the identification of the first liquid peak position along the Hugoniot, up to 4 Mbar. The time resolution shows ultrafast (between several tens and several hundreds of picoseconds) solid-solid and solid-liquid phase transitions.

References:
[1] A. Krygier et al., submitted, (2018).

ON THE TRAIL OF URANUS' AND NEPTUNE'S DIAMONDS VIA LABORATORY EXPERIMENTS USING LASER INDUCED SHOCK COMPRESSION

Anja K. SCHUSTER (HZDR/ TU Dresden)

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KLEMMED, Benjamin (TU Dresden) TOIMIL-MOLARES, Maria Eugenia (GSI)
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TURNER, Sally J. (UC Berkeley) ZETTL, Alex (UC Berkeley)
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From the exploration of the ice giants Uranus and Neptune through NASA's Voyager 2 mission in the 80s and telescopes we learned, that their stratosphere comprises hydrocarbons [1, 2, 3]; methane and its photochemical products in mixing ratios depending on season, latitude and pressure [4]. In the planets' interior the high-pressure (100s of GPa), high- temperature (1000s of K) conditions are believed to lead to further chemical reactions for example polymerisation of methane into heavier hydrocarbons or hydrocarbon separation in the warm dense matter regime into diamonds and hydrogen [5, 6, 7]. Indeed, hydrogen at these conditions is supposed to be metallic [8] and the diamonds are assumed to precipitate towards the planets' centre. Using high intensity lasers, materials can be driven to such extreme conditions on a nanosecond timescale in the laboratory via shock compression. As demonstrated in previous pump-probe experiments using polystyrene (CH) targets, nanodiamond formation was observed (~5000K, ~150GPa) via in situ femtosecond X-ray diffraction [5, 6]. In order to better understand the diamond formation process, we work on recovering the nanodiamonds for post analysis. Therefore, several types of well-known and novel materials were tested for their capability of catching warm, dense hypervelocity particles after shock breakout preferably intact - amongst them inorganic aerogel types with different mechanical properties [9]. The capturing process itself is highly complex. It includes viscous drag, ablation, compression, thermal effects such as vaporization and melting of either the catcher or projectiles or both [10]. After recovery the impacted catchers were scrutinized following different strategies. The aerogel samples for instance underwent distinct chemical treatments – acidic or basic - to dissolve the aerogel matrix, such that the residual solution could be used for further analysis techniques. First results from Raman spectroscopy, X-ray diffraction and transmission electron microscopy yield promising but not yet fully conclusive evidence for recovered nanodiamonds. The current status of the diamond recovery project will be presented. Further steps and potential conclusions for our understanding of chemical reactions inside the icy planets will be discussed.

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AB INITIO STUDY OF MAGNESIUM OXIDE PROPERTIES UNDER SUPER-EARTH INTERIOR CONDITIONS

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Super-Earth-type planets remain very poorly constrained regarding their bulk composition, formation scenario, let alone their habitability. For instance, it is uncertain whether they have a convective mantle like the Earth. It is also unclear if their mantle is insulating or conducting. In the latter case the mantle could generate a magnetic field via dynamo processes. In order to better understand the properties of silicate materials under pressure- temperature conditions relevant for Super-Earth interiors, we studied MgO, one silicate end-member, with ab initio simulations based on density functional theory. We explored its phase diagram and complete equation of state. We also determined its electronic transport properties, conductivity and reflectivity, to characterize its behavior in the different phases. We find that liquid and solid MgO behave differently, and discuss the consequences for the planetary interiors.

STRUCTURAL STUDIES OF MINERALS AND COMPOUNDS AT PRESSURES ABOVE 200 GPA

Leonid DUBROVINSKY (Bayerisches Geoinstitut, University of Bayreuth)

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Laser heating techniques in diamond anvil cells (DACs) cover a wide pressure-temperature range – above 300 GPa and up to 5000 K. Recent advantages in on-line laser heating techniques resulted in a significant improvement of reliability of in situ X-ray powder diffraction studies in laser-heated DACs, which have become routine at a number of synchrotron facilities including specialized beam-lines at the 3rd generation synchrotrons. However, until recently, existing DAC laser-heating systems could not be used for structural X-ray diffraction studies aimed at structural refinements, i.e. measuring of the diffraction intensities, and not only at determining of lattice parameters. The reason is that in existing DAC laser-heating facilities the laser beam enters the cell at a fixed angle, and a partial rotation of the DAC, as required in monochromatic structural X-ray diffraction experiments, results in a loss of the target crystal and may be even dangerous if the powerful laser light starts to scatter in arbitrary directions by the diamond anvils. In order to overcome this problem we have developed a portable laser heating system and implement it at different diffraction beam lines. We demonstrate the application of this system for simultaneous high-pressure and high-temperature powder and single crystal diffraction studies using examples of studies of chemical and phase relations in the Mg-Fe-O and Fe-N systems, transition metals carbonates, and silicate perovskites.

MASS-RADIUS RELATIONS OF ROCKY EXOPLANETS AND THE B1-B2 MANTLE PHASE TRANSITION OF FERROPERICLASE (MG, FE)O

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PADOVAN, Sebastiano (DLR, Berlin, Germany)
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We calculate mass-radius relations based on structural models of low-mass solid planets of less than ten Earth masses using equations of state valid in the high-pressure limit for the radial density distribution. To partly overcome inherent non-uniqueness problems, we additionally calculate the fluid Love numbers $k_{n,f}$ for spherical harmonic degrees $2 <= n < 4$ [1], which are a measure for central mass concentration and, therefore, relevant for determinations of rotationally and tidally induced planetary shape parameters and light curve variations [2] and transit timing variations [3]. We assume super-Earth planets that are subdivided into an iron core and overlain by an MgO-rich mantle and investigate the sensitivity of $k_{n,f}$ to the structural phase transition from the cubic B1 (NaCl-type) structure to the B2 (CsCl-type) phase of ferropericlase (Mg,Fe)O at mantle pressures above 500 GPa [4]. The preliminary calculations of the resultant mass-radius relations suggest that this structural phase transformation would be most relevant for relatively massive rocky exoplanets with small iron cores due to the small density contrast between the B1 structure and the B2 phase. Whereas planets with radii above 1.45 times that of the Earth are likely to harbor the B2-MgO mantle phase, the existence of the B2-MgO mantle phase for planets as massive as 3 Earth masses is only possible if their central iron cores were sufficiently small. In turn, more massive planets could possess larger iron cores and still maintain the B2-MgO phase in their mantles [5].

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Session IV – Rocky Planets and their Evolution

MAGMA OCEAN CRYSTALLIZATION AND TERRESTRIAL PLANETS DYNAMICS

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The early life of terrestrial planets is characterized by strong energy releases related to accretion and differentiation processes as well as the presence of highly energetic, short-lived radiogenic isotopes. Under these conditions enough heat can be released to melt partially or entirely the silicate mantle of terrestrial bodies, thus forming magma oceans. The subsequent cooling and solidification of such magma oceans shapes the initial conditions of the long-term dynamics of the planetary mantle. Widely accepted fractional crystallization models of magma oceans predict a gravitationally unstable density configuration at the end of solidification, followed by a whole-mantle overturn. In contrast we show that the onset of solid-state convection in the cumulates pile underlying a magma ocean during the solidification can stir and homogenize the mantle to a large extent. In the case of a protracted magma ocean solidification, for example if the magma ocean is thermally blanketed by a flotation crust (the most widely accepted scenario for the lunar magma ocean) the production of secondary melts in the cumulates and their extraction into the magma ocean can significantly prolong its lifetime. For large bodies like the Earth or Venus, a better knowledge of the melting behaviour as well as phase transitions at large depths is essential to constrain this crucial event in the planetary evolution. This work is supported by Helmholtz Association (grant VH-NG-1017).

VOLATILE DEGASSING AND CHEMICAL SPECIATION OF THE C-O-H SYSTEM IN THE EARTH MAGMA OCEAN SCENARIO

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Frank SOHL (DLR Institute of Planetary Research)

During the early phase of its evolution the Earth was likely characterized by the presence of a magma ocean or several large magma ponds. In this period there was a strong interaction between the interior differentiation process, the silicate melt phase and the atmosphere. The aim of this research is to investigate the degassing of volatiles in the C-O-H system in the presence of a magma ocean and the subsequent development of the early Earth's atmosphere. The volatile outgassing and the chemical speciation were investigated throughout numerical model simulations. Specifically, we analyze the volatile transition from the mantle to the atmosphere by using the "Equilibrium and mass balance method". The most representative reactions for the outgassing process are simulated at pressures, temperatures and redox states which are characteristic for the magma ocean scenario. The gas chemical speciation is deeply influenced by both the thermodynamic properties and the redox state. In a reduced ambient and for low temperatures the main gas species are: CO, CH_4 and H_2. On the other hand in oxidizing condition the principal gas species are H_2O and CO_2. In addition, the pressure played a central role during the evolution of the magma ocean and the crust formation. The pressure has a strong effect on the solubility of the gas phases within the silicate melt and the related availability of outgassed volatile species. Lastly, considering an extension of the present scope, this analytical technique has the potential also to characterize the volatile behavior of planetary bodies subject to high internal pressures such as massive solid exoplanets. This work was funded by the DFG (SFB-TRR 170 "Late accretion onto terrestrial planets (LATP)", subproject C5).

STRATIFICATION OF MERCURY'S CORE

Marie-Hélène DEPROOST (Royal Observatory of Belgium)

RIVOLDINI, Attilio (Royal Observatory of Belgium)
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Like the Earth, Mercury has a global magnetic field, generated in its iron-rich liquid core. Thermal evolution studies of Mercury indicate that the present-day heat flow at the core mantle boundary is sub-adiabatic. This suggests the presence of a thermally stratified layer in the upper core. In this work, we use a coupled thermal evolution model of the core and the mantle to assess the conditions of occurrence of a thermally stratified layer at the top of Mercury's core and its effect on inner core evolution and dynamo action.

CONSTRAINTS ON THE LUNAR CORE COMPOSITION AND THERMAL STATE FROM GEOPHYSICAL DATA AND THERMODYNAMIC PROPERTIES OF LIQUID IRON-SULFUR ALLOYS

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A precise knowledge of thermodynamic properties of the lunar core is of prime importance for the ongoing efforts to reanalyze Apollo seismic data, for the interpretation of results from GRAIL and future projects to send seismometers to the lunar surface, and for understanding the thermal evolution of the Moon. Here we present a coherent thermodynamic model for liquid Fe-S alloys that is based on melting and recent thermoelastic data. From this model, densities and seismic velocities of liquid Fe-S alloys are calculated and liquidus temperatures are determined. We apply our model to infer the composition and present-day temperature of the lunar core from recent geodesy data by assuming a mantle density distribution deduced from lunar seismic data. Additionally we study the effects of our model on the thermal evolution of the core and evaluate the core's capacity to generate a magnetic field.

Session V – DAC Techniques and Applications

SIMULATING THE EFFECTS OF SHOCK COMPRESSION IN DYNAMIC DIAMOND ANVIL CELL EXPERIMENTS

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Shock compression results in the most extreme deformation conditions of materials with strain rates on the order of 10^4 - 10^{10} s^{-1}, pressures reaching up to several Mbars and shock and post-shock temperatures that can exceed the melting point. Several methods have been developed to experimentally generate shock waves using high-explosives, gas guns, electric discharge devices and lasers. The pulse length in these shock experiments ranges usually from μs to fs. This short time scale has in the past prevented in situ measurements of the structural changes of materials under compression and the interpretation of the shock- induced modifications relied thus largely on the study of the final decompressed material. With the availability of free electron lasers this has changed. Nevertheless, the compression effect that takes place during large impacts with pulse lengths up to seconds cannot be simulated with the above techniques. To circumvent this problem, dynamic diamond anvil cell experiments are currently tested on synchroton facilities such as DESY for their ability to simulate the effects of shock compression. In such experiments, samples are rapidly compressed with rates of several kbars per second, while X-ray diffraction patterns are recorded simultaneously. Although shock waves cannot be produced in dynamic DAC experiments, they have proven to reproduce characteristic shock effects in oxide and silicate minerals such as amorphization and high- pressure phase transformations [1,2]. The talk is intended to give an overview of the status quo, pitfalls and perspectives of dynamic diamond anvil cell experiments based on instructive examples of selected minerals.

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THE DYNAMIC RESISTIVE-HEATED DIAMOND ANVIL CELL: COMPRESSION UNDER CONTROLLED COMPRESSION RATES AND HIGH TEMPERATURES

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Dynamic compression experiments performed using diamond-anvil cells combined with piezoelectric actuators (dDAC) has become a powerful technique since it enables the study of a variety of samples under controlled compression rates. The dDAC bridges the experimental compression rate gap between static compression techniques and highly dynamic approaches employing flyer plates, gas guns or laser shocks. In the last years, we have developed our own dDAC setup at the Extreme Conditions Beamline (ECB) at DESY in collaboration with Lawrence Livermore National Laboratory (LLNL). This setup is based on the design described in Evans et al. 2007 [1] and consists of a hardened steel body that encloses both the piezoelectric actuator and the DAC. The employed piezoelectric actuator is capable of achieving its maximum expansion in 2.5 milliseconds, allowing for rapid compression of a sample in the DAC. By changing the voltage-time-path, the maximum applied voltage to the piezo, as well as the diamond culet sizes, we can vary the compression rates and peak pressures that can be achieved in the experiment. The combination of the dDAC with extremely sensitive GaAs LAMBDA detectors available at the ECB facilitates time-resolved x-ray diffraction measurements and enables dynamic characterization of crystalline materials on the millisecond timescale. We tested the dDAC setup on polycrystalline MgFeO, where we realized compression rates of hundreds of TPa/s across the iron spin transition, while simultaneously collecting x-ray diffraction data. Furthermore, a dynamic resistive-heated DAC (dRHDAC) has been developed at the ECB to facilitate dynamic compression at high temperatures. It is based on the design described in Du et al. 2001 [2] and consists of two rigid graphite heaters that surround the gasket. The dRHDAC has recently been employed at the ECB to carry out dynamic compression experiments on H_2O ice VII at 800 K. In these experiments, we have collected 60 pressure points along the isotherm from 6 to 36 GPa in 1 minute. Here, we will discuss the experimental dDAC setup as well as first results and future perspectives.

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NEW DESIGN OF DOUBLE-STAGE DIAMOND ANVILS SHAPED FROM SINGLE CRYSTAL DIAMOND PLATE

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The invention of diamond anvil cell (DAC) in 1959 made it possible to explore extreme energy-density regimes. In particular, DACs found many applications in geophysics and planetary sciences as they allow simulating pressure and temperature conditions of planetary interiors in the laboratory. Among a number of static high-pressure apparata, diamond anvil cells can provide the capability of a wide range of in situ measurements covering the conditions over the entire Earth interior. However, achieving pressures over 150 GPa, is still very challenging. In order to reach higher pressures, the design of DACs went through a number of steps of development, such as, for example, the introduction of beveled diamond anvils and other refinements of the anvil shapes leading eventually to a multi-anvil geometry. The aim of this work was the fabrication and evaluation of capabilities of the secondary anvils of the new design to be used in the double-stage DACs (dsDACs). Micron-sized diamond anvils were produced from a single-crystal diamond plate using a focused ion beam (FIB) system. A sandwich-type secondary anvil consists of two diamond disks with the diameter of 20 μm and the thickness of 10 μm. Internal gasket was made of a pre-indented Re-foil using preparation technique for TEM-samples to avoid the variation of thickness. Micro-manufacturing using a dual-beam FIB enables us to control anvils' shape, to put a sample exactly between the secondary-stage anvils and to assemble the secondary-stage anvils inside the FIB chamber, thus solving the problem of the otherwise difficult alignment. In order to evaluate pressure, dsDAC was loaded with a piece of a foil of gold, for which the equation of state is established up to 600 GPa by means of X-ray diffraction (XRD). Paraffin oil was used as a pressure transmitting medium. In situ high pressure XRD studies show that dsDACs with the sandwich-type secondary anvils were able to generate pressures over 180 GPa with primary anvils with the culet diameter of 250 μm. XRD experiments were conducted on the Extreme Conditions Beamline P02.2 at PETRA III, DESY, Hamburg, Germany (Perkin Elmer detector, λ = 0. 48488 Å).

TOROIDAL DIAMOND ANVILS FOR STATIC COMPRESSION EXPERIMENTS BEYOND 5 MEGABAR

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The diamond anvil cell has been around for over 50 years and has been the primary tool for routinely studying materials up to pressures of ˜3 Mbar. Experiments over 4 Mbar with in situ pressure determination have been reported, however these reports are scarce. This indicates that these experiments are challenging, and that the success rate of these experiments is quite low. However, critical for developing accurate fundamental physics and chemistry models, with possible applications in modeling interiors of large planets. In this presentation I will show that focused ion beam crafted toroidal single-crystal diamond anvils with ˜9.0 μm culets are capable of producing pressures over 5.0 Mbar. The toroidal surface prevents gasket outflow and provides a means to stabilize the central culet. We have reached a maximum pressure of ˜6 Mbar using Re as in-situ pressure marker, a pressure regime typically accessed only by double-stage diamond anvils and dynamic compression platforms.

Session VI – Gas Giants

THE INTERIOR OF JUPITER

Ravit HELLED (Institute for Computational Science, Center for Theoretical Astrophysics & Cosmology)

Probing the interiors of Jupiter is not an easy task. It requires a set of accurate measurements combined with theoretical models that are used to infer the planetary composition and its depth dependence. Jupiter consist of mostly hydrogen and helium; it is the mass of heavy elements that is not well determined, as well as their distribution within the planet. While the heavy elements are not the dominating materials in Jupiter they are the key for our understanding of Jupiter's formation and evolution history. The planetary internal structure is inferred from theoretical models that fit the available observational constraints by using theoretical equations of states (EOSs) for hydrogen, helium, their mixtures, and heavier elements. However, there is no unique solution for the planetary structure and the results depend on the used EOSs and the model assumptions imposed by the modeler. Major model assumptions that can affect the derived internal structure include the number of layers, the heat transport mechanism within the planet, the nature of the core, and the location and degree of separation between different layers. The fact that the behaviour of hydrogen at high pressures and temperatures is not perfectly known, and that helium may separate from hydrogen at the deep interior add sources of uncertainties to structure models. Today, with accurate measurements of the gravitational fields of Jupiter and Saturn from the Juno and Cassini missions, structure models can be further constrained. At the same time, these measurements introduce new challenges for planetary modelers. In this talk, I summarise the current knowledge of the internal structure of Jupiter and the main open questions. The link to high pressure calculations and experiments will also be presented.

THE INTERIOR OF JUPITER WITH JUNO CONSTRAINTS: IMPORTANCE OF EQUATIONS OF STATE

Tristan GUILLOT (OCA)

Juno has provided extremely accurate constraints on Jupiter's gravity field. This implies that strong constraints on the depth of the planet's zonal flow can be inferred, solving a 40-year old puzzle [1]. The task is now to constrain the composition and internal structure of the giant planet. I will show that a significant issue remains the behaviour of hydrogen and helium in a regime between at 100 kbar to 10 Mbar (10 to 1000 GPa) and temperatures between 3000 and 20 000K. In this regime, similar ab-initio equations of state predict different interior model solutions [2]. Furthermore, the situation for the hydrogen-helium mixture appears more puzzling: The latest, most up-to-date calculations predict no phase separation of helium in Jupiter [3], when the Galileo probe measured an abundance of helium that is significantly lower than the protosolar value. Combined work on high pressure physics and interior models will be crucial to improve our understanding of the largest planet in the solar system, and beyond the origin of the solar system itself.

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DYNAMO ACTION OF JUPITER'S ZONAL FLOWS

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The new data delivered by NASA's Juno spacecraft significantly increase our understanding of Jupiter's internal dynamics. While Juno's magnetometer reveals the internal magnetic field, the gravity data constrain the depth of the zonal flows, which seem to slow down considerably at about 0.96% of the planet's radius. Here we study the possible dynamo action of the zonal winds. In a first step, we explore numerical dynamo simulations that incorporate a Jupiter-like electrical conductivity profile, concentrating on the region where the electrical conductivity decreases steeply with radius. The simulations show that the dynamo action obeys a simple quasi-stationary dynamics. Locally induced magnetic field and electrical currents can therefore reasonably be estimated based on three ingredients: 1) a surface field model, 2) an electrical conductivity model, and 3) a flow model. In a second step, we apply our findings to Jupiter, using the new magnetic field model JRM09, three different zonal flow models, and two suggested electrical conductivity profiles. Estimates of the electric currents allow predicting the entropy production due to Ohmic heating, which cannot exceed the entropy flux out of the planet. This provides a new constraint on the depth profile of the zonal flows and on the electrical conductivity profile. When, for example, using the conductivity suggested by [1] the zonal winds cannot reach below 0.955% of Jupiter's radius with undiminished speed. The locally induced radial field reflects the zonal flow structure. Reaching amplitudes of at least 10^{-6} Tesla, it should thus be detectable by the Juno magnetometer.

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Session VII – XFELs and Shock Methods

MEASURING PLASMA PARAMETERS OF WARM DENSE MATTER FROM X-RAY THOMSON SCATTERING AT THE LCLS AND THE NIF

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V. RECOULES (CEA,DAM,DIF)
P. SPERLING (SLAC National Accelerator Laboratory, European XFEL, Holzkoppel)
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The thermal and electrical conductivity, equation of state and the spectral opacity in warm dense matter (WDM) are essential properties for modeling, e.g., fusion experiments or the evolution, interior and magnetic field generation of planets. In the last decade it has been shown that x-ray Thomson scattering (XRTS) is an effective tool to determine plasma parameters like temperature and density in the WDM regime [1]. Recently, the electrical conductivity was extracted from XRTS experiments for the first time [2]. The spectrally resolved scattering data of aluminum, isochorically heated by the Linac Coherent Light Source (LCLS), show strong dependence on electron correlations. Therefore, the damping of plasmons, the collective electron oscillations, has to be treated beyond perturbation theory. Furthermore, an ongoing experimental campaign at the National Ignition Facility (NIF) measures XRTS spectra of imploding beryllium capsules for the first time in forward direction under extreme conditions, i.e. beyond 20 times compression. Here, we present results for the dynamic transport properties in warm dense aluminum and beryllium using density-functional-theory molecular dynamics (DFT-MD) simulations. The choice of the exchange-correlation (XC) functional, describing the interactions in the electronic subsystem, has significant impact on the ionization energy of bound electrons and the dynamic dielectric function. Our newly developed method for the calculation of XRTS signals including plasmon and bound-free transitions is based on transition matrix elements together with ionic contributions using uniquely DFT-MD simulations. The results show excellent agreement with the LCLS data if hybrid functionals are applied [3]. The experimental finding of nonlinear plasmon damping is caused by the non-Drude conductivity in warm dense aluminum. Here, we show further validation by comparing with x-ray absorption data [4]. These findings enable new insights into the impact of XC functionals on calculated properties of WDM and allow detailed predictions for ongoing experiments at the extreme densities reached at the NIF [5].

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RAPID TARGET HEATING WITH HIGH INTENSITY XFEL BEAMS

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Direct heating by hard X-ray irradiation ($E\gamma \approx 10$ keV) has only relatively recently become possible, with the advent of X-ray Free Electron Lasers (XFELs). Compared to approaches such as optical laser irradiation, or charged particle heating, it offers a variety of advantages in terms of being fast, isochoric and volumetric [1]. However, it proceeds mostly by exciting high-energy photo- and Auger electrons, the subsequent relaxation of which is complex to model, and which tends to heat a much larger region of the sample than the irradiated spot [2]. In this talk, we will present results from the Japanese XFEL SACLA (SPRing-8 Angstrom Compact free electron LAser). Various samples, both metallic and non-metallic, were irradiated by 9.8 keV X-ray photons with an incident intensity on the order of 10^{20} W/cm^2, by using the Kirkpatrick-Baez focusing mirrors to give a spot size of around 200 nm. The heated samples were subsequently probed by a second pulse, to observe changes in the diffraction pattern at a delay of up to 300 fs [3], and the samples examined by optical and scanning electron microscopes after the beam time. The results are varied, with some samples showing no damage while in others, the onset of rapid disordering is observed. We will discuss reasons for these differences, as well as future experiments and diagnostics, both at SACLA and at the new European XFEL.

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STUDIES OF MATTER AT EXTREME CONDITIONS USING HARD X-RAY FELS

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With availability of FELs in the hard X-ray regime, novel ways of studying matter at extreme conditions become feasible. The short pulse length of FELs allow to take snapshots of - extremely short lived states of matter and enables to study matter at conditions relevant for astrophysics and planetary sciences. With the principle of pump-probe experiments, electronic and structural reactions of materials can be studied with a time resolution down to femtoseconds, much shorter than a phonon period. So far the relevant conditions of pressure and temperature at FELs can either be reached by the XFEL directly causing isochoric heating of the material or by long pulse optical lasers that generate dynamic compression in the sample at strain rates of typically 10^4 - 10^7 s^{-1}. The high energy density science instrument (HED) at European XFEL will enter user operation in early 2019 and will make a high power optical long pulse laser for dynamic compression experiments available for experiments from late 2019. X-ray techniques to study the samples at extreme pressures and temperatures include spectroscopy and imaging methods as well as diffraction. The unprecedented brightness offered by European XFEL at hard X-ray energies up to 25 keV facilitates method development utilizing diamond anvil cells (DAC). The combination of rapid compressions and pulsed laser heating with DAC technology opens up the capability to create extreme states in matter, which are short lived and therefore require fast probing by the FEL X-ray pulses. Besides classical pump-probe techniques, the X-ray repetition rate of European XFEL of up to 4.5 MHz can be employed to record a movie of the evolution of these extreme states with up to 220 ns time resolution. In this contribution, we present recent examples of planetary science studies using XFELs and will describe the type of science that can be addressed by the new developments. In addition, we will show the current design and the implementation of the experimental setups and update on the status of the HED instrument.

POLYMORPHISM, AMORPHIZATION AND MELTING OF SIO$_2$ AND MG-BEARING SILICATES FROM IN-SITU X-RAY DIFFRACTION OF LASER-DRIVEN SHOCK-COMPRESSION

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Riccardo BOLIS (Ecole Nationale Superieure d`Arts et Metiers, France)
Arianna Elizabeth GLEASON (SLAC National Acceleration Labatory, Stanford University)
Roberto ALONSO MORI (SLAC National Acceleration Labatory, Stanford University)
Norimasa OZAKI (Osaka University)
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The determination of terrestrial planets structure and evolution and the understanding of impact metamorphism rely on the phase relations in the Mg-Si-O ternary system at extreme conditions of pressure and temperature under various rates of compression. In December 2017 we performed in-situ X-ray diffraction (XRD) measurements of laser-shocked SiO$_2$, MgSiO$_3$, Mg$_2$SiO$_4$ glass and crystalline phases at the MEC end-station of the LCLS facility at SLAC (Standford, USA). We investigated pressures up to few Mbar along the principal Hugoniot. Here, I will present an overview of the results, including evidences of polymorphism, amorphization and melting. In particular, at increasing pressures along the Hugoniot, we found that fused SiO$_2$ first forms a dense amorphous phase and then directly crystallizes into stishovite whereas alpha-quartz first undergoes a single-crystal-to-single- crystal polymorphic transition prior to the high-pressure stishovite crystallization. MgSiO$_3$ glass presents a structural evolution consistent with high-pressures, high-temperatures static experiments and does not crystallize in bridgmanite or post-bridgmanite below the melting temperature. Shocked enstatite single crystals also undergo a single-crystal-to-single-crystal transition and amorphize at higher pressures. Shocked forsterite produces complex single crystal diffraction patterns showing anisotropic deformations. Again we do not find any evidence for dissociation into MgSiO3 + MgO at higher pressure prior to melting. Such results have implications on the formation of impact glasses, and on the use of silicate glasses as analogues of silicate melt.

Session VIII – Molecular Systems II

THEORY AND SIMULATIONS OF THE COMPRESSIVE FREEZING TO ICE VII

Jonathan BELOF (Lawrence Livermore National Laboratory)

The metastability and kinetics of non-equilibrium phase transformations in water present one of the greatest mysteries of condensed matter physics and chemistry. Owing to its unique inter- and intra-molecular interactions, water is likely the most polymorphic material in existence – having over 17 ice phases, most of which are accessible only at high pressure. Developing an understanding of the nucleation of ice at high pressure has direct implications for the origins of life on extrasolar "super-earths", ocean worlds that have been detected by the Kepler telescope. Over the years, experiments that solidify water into the high-pressure ice VII phase by application of pressure via dynamic DAC, pulsed-power and gas-gun platforms have presented seemingly contradictory results regarding the nucleation of ice far from equilibrium. Here we show that, under these extreme conditions, classical nucleation theory can successfully describe these freezing experiments but only if amended to include new aspects that are unique to the non-equilibrium state – transient nucleation and thermal disequilibrium between ice and liquid – and that by doing so we are able to reconcile the apparent discrepancies between various nucleation experiments. The role of the liquid-ice interface is highlighted in the current model and possible effects on nucleation from quantum motion of the proton/deuteron are also predicted.

PROTON DYNAMICS IN HIGH-PRESSURE ICE-VII FROM DENSITY FUNCTIONAL THEORY

Florian TRYBEL (Bayerisches Geoinstitut)

Gerd STEINLE-NEUMANN (Bayerisches Geoinstitut)
Thomas MEIER (Bayerisches Geoinstitut)

The recent discovery of natural ice-VII diamond inclusions [1] shows the importance of this high-pressure water phase not only as a purely physical phenomenon but also in the context of Earth's deep mantle and within the structural investigation of water-rich planets and moons in- and outside of our solar system. Ice-VII is a solid cubic phase of H_2O with a stability field of 2 to approximately 70 GPa at 300 K [2]. Within the body centered cubic (bcc) oxygen lattice two possible proton positions along the diagonal O-O direction exist and are randomly populated according to the ice-rules. At higher compression the structure undergoes a continuous phase transition to the symmetric ice-X phase [2]. The disorder in the proton positions and the related possibility of proton tunneling due to the occurrence of a double-well potential along the diagonal O-O direction as well as the high pressure symmetrization have been part of many studies. We present a method using low cost density functional theory (DFT) simulations to map out and investigate the double-well potential and related proton dynamics in ice-VII. In agreement with previous work we find a double-well potential along the diagonal O-O direction with the barrier height and minima distance decreasing with pressure. Consequently our calculations predict an increasing tunneling probability as well as the continuous phase transition to the symmetric ice-X phase in good agreement with the experimental NMR study [3].

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THERMAL CONDUCTIVITY OF WATER PLASMAS FROM AB INITIO SIMULATIONS

Martin FRENCH (Universität Rostock)

The determination of thermal conductivities of dense plasmas is a great challenge for both experimental and theoretical approaches. In partially ionized plasmas, not only electrons contribute to the thermal conductivity but also ions. Here we use ab initio molecular dynamics (MD) simulations based on density functional theory (DFT) to calculate the ionic contribution to the thermal conductivity of dense partially ionized water plasmas. The required heat current of the ions is determined by matching the forces from each of the DFT-MD simulations onto effective pair interaction force fields. These force fields are then used to evaluate the Green-Kubo relation for the thermal conductivity using the ion trajectories of the same DFT-MD simulation run. This approach is generally applicable to various multi-component plasmas as well as to materials in liquid, solid, or superionic phases. For water plasmas the ionic contribution to the thermal conductivity is found to be equal to or greater than the electronic contribution [1] up to temperatures of 20 000 K, depending on the density. The presence of characteristic contributions from thermal dissociation reactions of the water molecules can be traced back to the shapes of the derived force fields between the ionic species. These contributions enhance the ionic thermal conductivity between 3000 and 10 000 K noticeably and are more pronounced toward low densities. Additional benchmark calculations for ice VII and liquid water show good agreement with experimental data and with an ab initio study in which the ionic heat current was determined with a generalized variant of density functional perturbation theory for the electronic ground state [2]. Our results are of general significance for understanding thermal transport properties in dense, partially ionized plasmas and other states of matter. The generated thermal conductivity data for water are particularly important for the development of non-adiabatic evolution models for water-rich giant planets like Uranus and Neptune. This work is supported by the DFG within the FOR 2440 "Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics."

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Poster Session

ELECTRONIC STOPPING POWER OF WARM DENSE MATTER FROM TDDFT - EHRENFEST DYNAMICS

Wildan ABDUSSALAM (Helmholtz Zentrum Dresden Rossendorf)

VORBERGER, Jan (HZDR)

The electronic stopping power is important quantity in the study of warm dense matter as it plays an essential role in the processes depositing energy into the system. More specifically, these are essential for creating such warm dense states in the laboratory and for applications in fusion energy or medicine. Conventional theoretical models based on kinetic approaches have difficulties in simultaneously including essential warm dense matter features such as strong coupling, collective effects, and quantum effects. Here, we present first results of the stopping of protons in boron based on time-dependent density functional theory and Ehrenfest dynamics. We demonstrate good agreement with experimental results for room temperature and show how this method can be used for warm dense matter states for validation and benchmarking.

NANOSECOND FREEZING OF WATER NEAR THE METASTABILITY LIMIT

**Jonathan BELOF** (Lawrence Livermore National Laboratory)

The fundamental study of phase transition kinetics has motivated experimental methods toward achieving the largest degree of undercooling possible, more recently culminating in the technique of rapid, quasi-isentropic compression. This approach has been demonstrated to freeze water into the high-pressure ice VII phase on nanosecond timescales, with some experiments undergoing heterogeneous nucleation while others, in apparent contradiction, suggest a homogeneous nucleation mode. In this study, we show through a combination of theory, simulation, and analysis of experiments that these seemingly contradictory results are in agreement when viewed from the perspective of classical nucleation theory. We find that, perhaps surprisingly, the classical nucleation theory is capable of accurately predicting the solidification kinetics of ice VII formation under an extremely high driving force ($\Delta\mu/kT \approx 1$) but only if amended by two important considerations: (i) transient nucleation and (ii) separate liquid and solid temperatures. This is the first demonstration of a model that is able to reproduce the experimentally observed rapid freezing kinetics.

DO IMPACTITES CONTAIN METAL CONDENSATE FROM EVAPORATED METEORITE?

Christian BENDER KOCH (Department of Chemistry, University of Copenhagen)

T. Kasami (CEN, Technical University of Denmark)

It is generally agreed that metallic meteorites may evaporate during the conditions of high-velocity impact. However, the detailed conditions and the resulting materials are only poorly understood. Morphological studies of impactites from the almost pristine impact craters at Wabar in Saudi Arabia, have revealed abundant vesicles having their inner curved surfaces decorated by metallic sphere-like particles. The spheres are commonly 1-2 my in diameter and occur in partially correlated deposit structures – most commonly in strings and never on-top or touching each other. The deposition of the spheres appear to have involved the imbedment into the hosting glass at a time where the glass was molten, thus implying that the spheres were correlated within the space of the vesicle. We suggest that the vesicle volume represent the volume of the hot, pressurized metal vapour prior to cooling followed by condensation the metal.
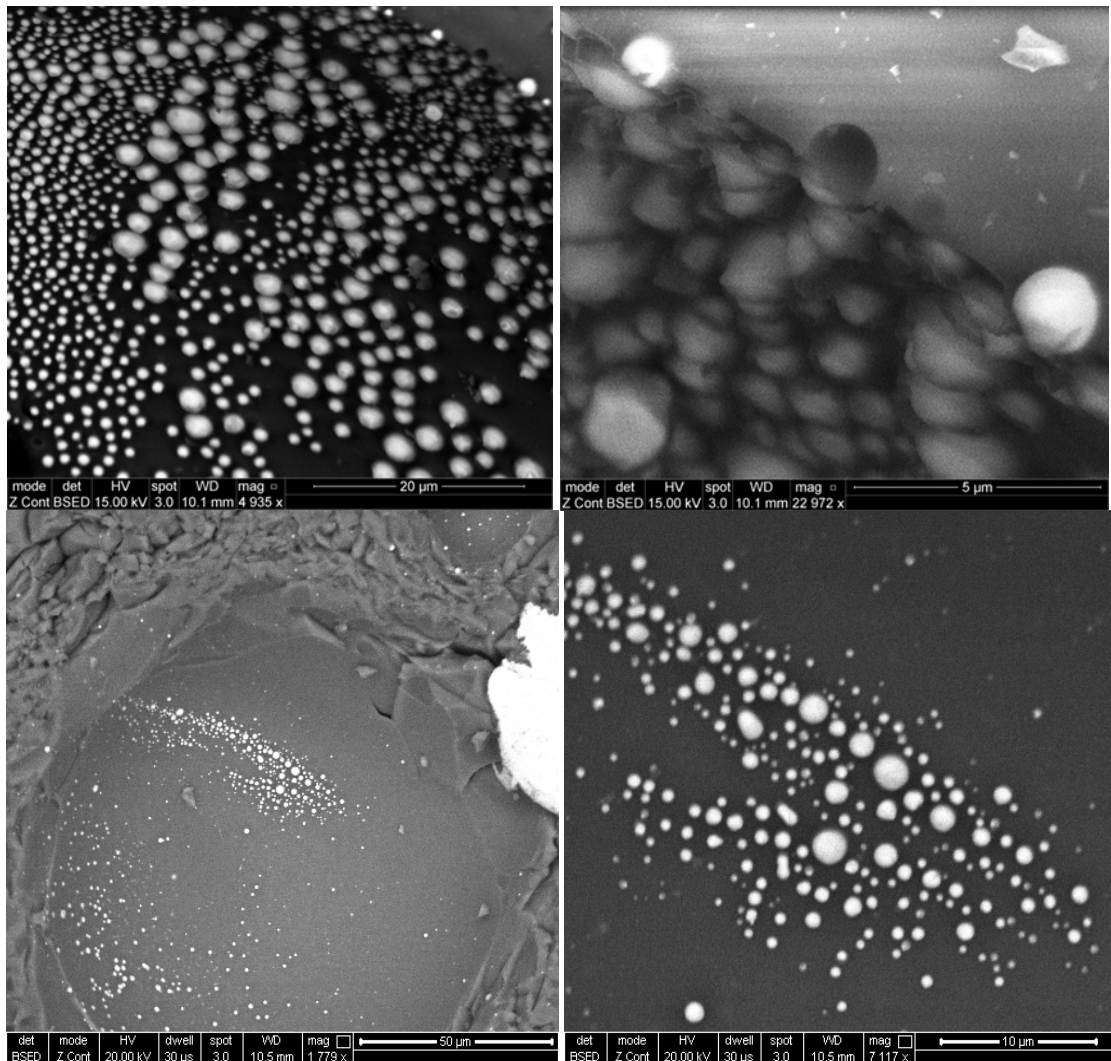
Upper left: A bimodal distribution of metal spheres (showing bright in the backscatter mode) decorating the inside of a vesicle. Upper Right: Detail of vesicle/glass transition showing spheres embedded in the glass and the imprint of a sphere that has been removed from its embedded position. Lower left: Vesicle exhibiting correlated and random deposition of metal spheres. Lower right: detail of correlated deposit.

DFT+U EQUATION OF STATE FOR IRON OXIDE

Daniel CEBULLA (University of Rostock)

Mandy BETHKENHAGEN (University of Rostock)
Ronald REDMER (University of Rostock)

The number of detected exoplanets and the capabilities of identifying small, Earth-sized planets have grown tremendously over the last two decades. Yet many of those Earth-sized planets are only characterized in mass and radius. Therefore, interior structure models rely heavily on equations of states (EOS) for rock material to characterize the planetary properties. One particular interesting material is iron oxide, which is very challenging to treat with standard Density Functional Theory (DFT) methods. Here we investigate the DFT+U approach to obtain the correct electronic and structural properties for the FeO phases typically predicted at the high pressures within the planetary interiors. The Hubbard U is obtained self-consistently from spin-polarized DFT calculations with QUANTUM ESPRESSO [1,2] using the linear response approach [3]. The resulting optimized ground state is used as a starting point for phonon calculations within the quasi-harmonic approximation. Based on these calculations we investigate the impact of the Hubbard U on the EOS providing a step forward to incorporating more realistic rock material into interior structure models of super Earths.

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LOVE-NUMBER OF WASP-18AB

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Alexis SMITH (Institute of Planetary Research, German Aerospace Center (DLR), Berlin, Germany)

Exoplanets and their host stars exhibit a mutual tidal interaction. One of the consequences of this phenomenon is the so-called apsidal motion: the major axis of the eccentric orbits rotate around the host star and it is called either apsidal motion or periastron precession. The rate of this precession linearly depends on the k_2 fluid Love-number of the planet and therefore this effect, when this motion is observable, provides an opportunity to measure it. Theoretical predictions suggest that WASP-18b is one of the systems which features the biggest apsidal motion rate which should be observable by radial velocities and by transit timing variations within a few years. We analyze the available archival radial velocity data and we are able to give limits for its Love-number.

MULTICOMPONENT MELTING IN A HETEROGENEOUS LUNAR MANTLE AFTER MAGMA OCEAN SOLIDIFICATION

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Ana-Catalina PLESA (German Aerospace Center (DLR), Berlin, Germany)
Sabrina SCHWINGER (German Aerospace Center (DLR), Berlin, Germany),
Yue ZHAO (Vrije Universiteit Amsterdam)
Doris BREUER (German Aerospace Center (DLR), Berlin, Germany)

The early stages of lunar evolution have been characterized by the cooling and crystallization of the Lunar Magma Ocean (LMO). The fractional solidification of the magma ocean led to the formation of an unstably stratified interior, which can largely affect the subsequent thermo-chemical evolution of the Moon. We model the thermo-chemical evolution of a compositionally heterogeneous Moon as a 2D quarter cylinder, using the convection code GAIA [1]. Conservation equations are solved using the Boussinesq Approximation. Our models start with a layered compositional structure as a result of the solidification of the LMO and includes ilmenite, olivine, orthopyroxene and clinopyroxene components. We use alphaMELTS [2] to calculate the post-crystallization temperature, the initial distribution of the components and their corresponding density. For the subsequent evolution, we calculate the melt fraction of the cumulates based on the individual solidus and liquidus temperatures of its components. This approach will provide a minimum melt estimate, as eutectic melting is not considered. We further include the effects of latent heat as in [3] and trace each component and its depletion, using a particle-in-cell (PIC) method as described by [4].

In this study, we investigate the first Gyr of the lunar thermo-chemical history after the crystallization of the LMO. This approach allows us to examine the effects of melting and depletion of various mantle components on the thermochemical evolution of the Moon. In the next stages, a more detailed approach to calculating solidus and liquidus temperatures considering the chemical mixing of components with advection and using appropriate solidus temperatures for eutectic melting could be used to yield maximum melt estimates. Furthermore, these simulations will be used as a basis for including additional compositional heterogeneities due to melting of the mantle produced by large-scale impacts or considering asymmetric initial conditions as in [5].

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ISOTOPIC SHIFT OF THE INSULATOR-METAL TRANSITION IN DENSE FLUID HYDROGEN

Rachel HUSBAND (DESY Hamburg)

The liquid-liquid insulator-metal transition in dense hydrogen (LLIMT) is of interest for both fundamental and planetary sciences. In gas giants, the LLIMT determines the boundary between insulating molecular and atomic metallic hydrogen, and as such it is an important feature in interior models of Jovian-like planets. In order to provide an insight into the importance of ion dynamics at the transition, it is useful to compare the behaviour of hydrogen with that of deuterium. However, almost all previous studies have treated hydrogen and deuterium without distinction. By studying the optical properties of statically-compressed deuterium, we have determined the metallization phase line in the 1.2 to 1.7 Mbar range. Compared to previous results on hydrogen collected using the same experimental technique, deuterium is observed to metallize at substantially higher temperatures than hydrogen at the same pressure. This reveals a prominent isotopic shift in the location of the phase lines. Interestingly, the temperature (energy) difference in the location of the phase transition lines of the two isotopes is comparable to the energetic difference in their free-molecule dissociation energies. These results highlight the importance of nuclear quantum effects in the hydrogen isotopes at these conditions, which should be accounted in future ab initio calculations.

IMPLEMENTATIONS OF DAC SETUP FOR DACS, DSDAC AND DDAC EXPERIMENTS AT THE HED INSTRUMENT OF THE EUROPEAN XFEL

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APPEL, Karen (HASY- LAB)
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DAMKER, Horst (DESY-ZM1)
FOESE, M. (DESY)
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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. These techniques may be used to determine Equation of State (EOS) and elastic properties as well as phase stabilities of different compounds at very high-temperatures and high-pressures. Thus, the combination of static DACs with isochoric x-ray or near infrared micro second laser heating does provide essential experimental data for e.g. the interpretation of the structure and dynamics of extra solar planets. 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/heating diffraction experiments are possible at 3rd generation sources up to the kHz (ms) regime, it will require new 4th generation sources, such as the European XFEL, to be able to conduct 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 with DESY as a strong partner. 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. Recently, the interested scientists from the high-pressure community have come together to propose first User Assisted Commissioning experiments to be conducted at the dedicated DAC setup for the HED instrument. Within this presentation we describe the current status of the construction of the DAC setup at the HED instrument as well as the first set of experiments to be conducted during commissioning or the user assisted commissioning proposal.

STATIC LOVE NUMBER K$_{NM}$ VALUES OF JUPITER FROM INTERIOR MODELS

Nadine NETTELMANN (University of Rostock)

The Juno spacecraft currently in orbit around Jupiter has provided a first estimate of the Love number k_2 of Jupiter [1]. Within the 10% observational uncertainty, the observed value of 0.625 is in agreement with computations of the static Love number k_2 from interior models of rotating Jupiter [2, this work] which predict a value of 0.589 with a possible range of about 0.2% only. The model computations are based on the CMS method for a rotationally and tidally perturbed fluid planet [3]. However, as the observational uncertainty in k_2 is decreasing with improving longitudinal coverage of Jupiter by Juno, it may be suspected that a gap may open between the computed static and the observationally determined values.

In this work I estimate the influence of Jupiter's four major satellites on Jupiter's static tidal response k_{nm}. I assume a linear super-position of the single satellite contributions. Inclusion of non-linear dynamic effects, which may have a larger influence on Jupiter's k_{nm} values, is left to future work.

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DFT CALCULATIONS OF THE LINEAR ELASTICITY OF QUARTZ AND IMPLICATIONS FOR PRESSURE-INDUCED LAMELLAR AMORPHIZATION

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LANGENHORST, Falko (Friedrich-Schiller-Universität Jena)

The transition of quartz to the amorphous state is a commonly observed phenomenon, when high pressures are rapidly applied at ambient temperature. Under shock compression, i.e. under the most extreme strain rates, quartz displays a peculiar amorphization behavior, as it develops amorphous lamellae at the nanometer scale with sharp crystalline-amorphous boundaries and most strikingly, along particular crystallographic planes. Here, we investigate the directional dependence of mechanical properties (Young and shear moduli) of quartz in the approximation of linear elasticity and compare our results with the orientations of amorphous lamellae. These calculations aim at gaining insight into their formation mechanism. We tackle the problem by calculating second-order elastic coefficients by means of density functional theory. Our first calculations of stress-strain relations for all directions indicate indeed structural changes over pressure that are consistent with anisotropic amorphization of quartz.

HIGH-PRESSURE BEHAVIOR OF FE$_4$O$_5$ AT LOW AND HIGH TEMPERATURES

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Elene BYKOVA (DESY)
Dr. GLAZYRIN (DESY)
Anna PAKHOMOVA (DESY)
Alexander KURNOSOV (Bayerisches Geoinstitut, Universität Bayreuth)
Valerio CERANTOLA (European Synchroton Radiation Facility)
Ilya KUPENKO (Institut für Mineralogie, Universität Münster)
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Iron oxides are fundamentally important materials for all basic sciences and technologies. The oldest known magnetic mineral, magnetite (Fe$_3$O$_4$) was the only simple mixed-valent iron oxide known until recently. It was discovered that near 120 K magnetite shows a metal-insulator-type transition (so-called Verwey transition), which was believed to be related to charge ordering [1]. Recently, the charge-ordering pattern in the Verwey phase of Fe$_3$O$_4$ was solved in single crystal X-ray diffraction experiments [2]. This study identified a novel type of 'quasi-particles' consisting of three iron ions with one shared electron (so-called "trimerons") [2]. In recent years several more mixed-valent simple iron oxides were discovered in high-pressure high-temperature conditions, corresponding to those in the Earth's interiors in the Upper and Lower Mantle, such as: Fe$_4$O$_5$ [3], Fe$_5$O$_6$ [4], Fe$_{13}$O$_{19}$ [5], Fe$_5$O$_7$ [6], Fe$_{25}$O$_{32}$ [6], FeO$_2$ [7], and Fe$_7$O$_9$ [8]. One of them, which is well quenchable at ambient conditions, Fe$_4$O$_5$ comprising mixed-valent iron cations at octahedral chains, demonstrates another unusual charge-ordering transition at 150 K involving competing formation of iron trimerons and dimerons [4]. In this work we synthesized large single crystals of Fe$_4$O$_5$ using multi-anvil high-pressure high-temperature synthesis facilities and investigated an effect of applied high pressure on the crystal structure and Mőssbauer spectra of this oxide. Some high-pressure experiments were carried out at low-temperature conditions, whereas, in the other runs we investigated the properties of Fe$_4$O$_5$ at room temperature before and after a laser heating of the sample. We found a number of structural phase transitions and designed a first pressure-temperature phase diagram of Fe$_4$O$_5$.

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SEISMIC VELOCITIES IN THE MARTIAN MANTLE AND CRUST CALCULATED FROM A 3D THERMAL AND MINERALOGICAL MODEL

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Doris BREUER (German Aerospace Center (DLR))
Tilman SPOHN (German Aerospace Center (DLR))

NASA's InSight (Interior exploration using Seismic Investigations, Geodesy and Heat Transport) Discovery-class mission will perform a geophysical investigation of Mars using a seismometer and a heat flow probe, as well as a precision tracking instrument. The seismic and heat flow data constrain the present-day interior structure and heat budget of the planet, and thus its thermal and chemical evolution [1]. As the InSight lander will perform measurements at a single location, in the Elysium Planitia region on Mars [2], 3D numerical simulations of planetary interiors will help to interpret the data in a global context.

In this study, we present 3D numerical thermal evolution models of Mars [3] and focus on the present-day state. We calculate seismic velocities from the 3D temperature data at present-day using the BurnMan code [4] with the Stixrude & Lithgow-Bertelloni 2011 mineral data base [5]. All our thermal evolution models use crustal thickness models derived from gravity and topography data and vary the following parameters: crustal enrichment in heat producing elements (HPE), crustal thermal conductivity, mantle reference viscosity, pressure-dependence of the viscosity, thermal expansivity, and core size. In particular, we investigate the consequences of various HPE distributions and crustal thickness models on the seismic velocity variations in the martian interior.

For a strongly enriched crust with an average thickness larger than 62 km, our models suggest a peak-to-peak difference in the P-wave velocity of up to 5% in the uppermost 400 km that correlates with the crustal thickness dichotomy. Estimates of the seismic velocity distribution in the lithosphere of Mars could be used to constrain the crustal enrichment in HPE.

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THE DYNAMIC DIAMOND ANVIL CELL (DDAC) AT THE HED INSTRUMENT OF THE EUROPEAN XFEL

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Experimental conditions reached by static high-pressure and high-temperature techniques utilizing diamond anvil cells and those that result from dynamically driven shock waves, such as in laser/magnetic or gas gun shock compression experiments, differ greatly in their thermodynamic pathways. Moreover, the two high pressure techniques yield very different strain rates whose impact on the physical properties of matter is unclear. A piezo driven dynamic DAC [1] is a technique developed to reach intermediate strain rates between those from static and dynamic compression. Higher compression rates, however, require use of fast X-ray probes, of high brilliance, and fast large area detectors for diffraction experiments – a unique combination offered by the High Energy Density (HED) instrument at the European XFEL [2]. The HED instrument will feature a second interaction chamber (IC2) with a setup dedicated to research using diamond anvil cells. With the unique hard energy X-rays (up to 25 keV) and high sampling rate (220 ns between two successive pulses), provided by the European XFEL, one can efficiently probe the structural properties of material as the stress state continuously increases up to the mechanical limit of the DAC. Here we present preliminary studies on fast compression of metals in membrane DAC conducted at the Extreme Conditions Beamline P02.2 of Petra III, DESY, Germany [3]. The materials of choice (Fe [4], Pt, RE, stainless steel) give us hint on microstrain behavior of the sample and gasket assembly during the compression/decompression ramps, which yields better understanding of sample preparation for future dDAC experiments. Further, we will show some capabilities of the dDAC techniques in terms of reachable compression rates and discuss further developments of these experiments at FEL sources. Our future plan is to explore the structural behaviour and properties of MgO, FeO and (Mg,Fe)O solid solutions (Fe% = 20, 40, 60, 80) at different strain rates and at multimegabar pressures. Dynamic DAC experiments combined with pulsed laser heating will enable us to cover large P,T space using an approach complementary to the static and dynamic techniques.
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THE MELTING LINE AND THE BAND GAP OF HELIUM

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We studied the behavior of solid and liquid helium under high pressure with molecular dynamics simulations based on density functional theory (DFT-MD). Helium, as the second abundant element in nature, is important for astrophysical applications, e.g., the interior and evolution of gas giants and brown dwarfs. In particular, we calculated the melting line and examine the insulator-to-metal transition, both for extreme pressures up to the TPa region. The calculation of the melting line is a challenging topic in computational physics. Out of many approaches of different complexity and efficiency, two-phase simulations represent a very intuitive approach with high accuracy [1]. We have implemented this method and investigated finite-size effects and other convergence issues. We found good consistency with available experiments and gave predictions for the melting line of helium up to the TPa region.

Laser-driven compression experiments have shown that helium undergoes an insulator-to-metal transition with increasing density and temperature [2]. However, the exact location and nature of this transition is not clear yet. The most recent publications on the calculation of closure of the helium band gap [3,4] differ within a factor of two in density and employ different definitions of the band gap. We performed extensive convergence tests and found good agreement with the results of [4].

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FIRST-PRINCIPLES STUDY OF THE ELECTRONIC STRUCTURE AND DIELECTRIC RESPONSE FUNCTION OF DIAMOND AND OTHER RELEVANT HIGH PRESSURE PHASES OF CARBON UP TO 15 MBAR

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The description of equation of state (EOS) and phase transitions requires state of the art ab initio methods such as density functional theory (DFT) with molecular dynamics, path integral Monte Carlo. The combination of DFT and many-body quantum statistics is to enhance accuracy, predictive power and to bring simulation and experiment closer together. The dynamic structure factor (DSF) is an important parameter to determine warm dense matter properties and can be accessed using x-ray Thomson scattering from energetic x-ray sources at LCLS, SACLA or EU-XFEL. Enhanced DSF models need the inclusion of electron-hole interaction in semiconductors/insulators along with higher rungs of exchange-correlation functionals. The consequences are better EOS models and temperature measurements through DSF. The electronic structure of diamond, body centered cubic diamond (bc8), hexagonal diamond (lonsdaleite) phases of carbon are computed using density functional theory and the optical response using many-body perturbation theory up to 15 Mbar with the emphasis on the excitonic picture of the solid phases relevant in the regimes of high-pressure physics and warm dense matter.

PARAMAGNETIC-TO-DIAMAGNETIC TRANSITION IN DENSE LIQUID IRON AND ITS INFLUENCE ON ELECTRONIC TRANSPORT PROPERTIES

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We calculate the electrical and thermal conductivity of liquid iron with spin-polarized density-functional-theory-based simulations over a significant pressure and temperature range using the Kubo-Greenwood formalism. We show that a paramagnetic state is stable in the liquid up to high temperatures at ambient pressure, and that the discrepancy between experimental results and spin-degenerate simulations for the conductivities of more than 30% are reduced to within 10% with lower values resulting from the spin-polarized simulations. Along the 3700 K isotherm, we explore the persistence of magnetic fluctuations toward high densities and beyond 20-50 GPa the liquid becomes diamagnetic. We predict a pronounced paramagnetic-to-diamagnetic transition, probably of second or higher order. This transition exerts a significant influence on the physical properties of liquid iron, especially on the conductivities, and is potentially of high relevance for dynamo processes in Mercury and Mars.

SYNTHETIC GEOPHYSICAL OBSERVABLES FROM MARTIAN MANTLE CONVECTION MODELS, WITH APPLICATION TO INSIGHT

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We model the thermochemical evolution of Mars with the fully dynamical mantle convection code STAGYY [1] coupled to a petrological and mineral physics model of the mantle and core materials to determine their physical properties and melting behavior (cf. [2]). Starting at 4.4 Ga, the models are allowed to evolve undergoing compositional changes due to melting and are subjected to a large, basin-forming impact at 4 Ga that causes further melting and heating of the mantle and introduce major thermal and compositional anomalies. The impacts are implemented in a simplified, parameterized form that focuses on describing the first-order effects caused by shock-heating in the surroundings of the impact site (e.g., [3]). The final result of a typical modeling run is a model of the present-day thermal and compositional state of the martian interior, in particular of the mantle. The coupling of the fluid-dynamical model to the mineral physics model allows to derive various geophysical observables from the model in an internally consistent way. Some of the most important physical properties are the density, the seismic velocities, and the thermal and electrical conductivity, which are observed by gravity, seismics, heat flow measurements, and magnetic observations from orbit or from the ground. Gravity and magnetic measurements of Mars have been carried out by spacecraft for many years, whereas seismic and heat flow observations as well as further magnetic data are expected to become available after 2018 with the deployment of the InSight lander now on its way to Mars. The increased depletion caused by impacts modifies the density of the target and thus leaves a low-density mantle anomaly that is expected to be visible in gravity measurements. The contributions of both the crust and the mantle to the total anomaly are detectable by ground-based and orbiting spacecraft and that neglecting the mantle anomaly may result in misestimates of the crustal thickness on the order of several kilometers. Seismic velocity models of the mantle reproduce the expected first-order seismic discontinuities of the martian interior, including a mid-mantle discontinuity of ~210 m/s at a depth of about 1100 km that is mostly due to the high-pressure phase transitions of olivine; shallow, impact-generated anomalies, however, are too small to be detected with single stations such as the SEIS experiment of InSight. Global heat flows from the models are consistent with the geochemical model by [4]. Local circumstances such as anomalous crustal properties in impact basins due to the deposition of cold crust at the surface result in heat flows that lie at most a few mW/m^2 below the global average. Modelled electrical conductivities tend to be lower than those derived from MGS data [5] so far and suggest a higher water content of the martian mantle than in the geochemical models mostly derived from shergottite compositions.

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THE MARTIAN DYNAMO POWERED BY FE SNOW

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Mars' strongly magnetized crust suggests that a core dynamo has been active in the past (4.1-3.7 Gyr ago) [1], but not a present day. A popular explanation for the observation is an early thermally driven dynamo and the absence of an inner core [2].

The feasibility of a present-day entirely liquid core, however, depends on the concentration of sulfur in the core, which is known to depress the liquidus temperature [3]. Chemical analysis of SNC (Shergotittes, Nakhlites, Chassignites) meteorites and an oxygen isotope model indicate the presence of 14.2 wt% [4] and 10.6 wt% [5] sulfur in the core, respectively. More recent geochemical analysis [6], however, indicates much lower sulfur concentrations (<5-10 wt.%) in the Martian core. Interpolation of experimental data [7] shows that the pressure slope of the Fe-FeS liquidus temperature is positive but shallow or even negative (xs>10 wt%) in Mars' core pressure range. As a consequence, core crystallization, if it occurs, most likely commences at the core-mantle boundary and proceeds in the Fe snow regime. The latter is characterized by a snow zone with "snowing'' iron crystals and an entirely liquid, convecting core below the snow zone. The snow zone grows with ongoing cooling until it covers the entire core and the crystals compact into a solid inner core. The dynamo in the Fe snow regime resides in the deeper, convecting core below the snow zone. It is known to be short-lived (< 1 Gyr) and its demise is associated with the occurrence of a solid inner core [8].

Fe snow in the Martian core has recently been investigated by [9]. The study concluded that snow zones thinner than 400 km are compatible with the absence of a present-day magnetic field. The study, however, focused solely on the core and did not consider the evolution of the overlying mantle. The latter is important in order to estimate the timing of the dynamo.

The present work attempts to investigate the timing of Fe snow in the Martian core and its compatibility with observations, i.e. an early magnetic field and absence of a present-day magnetic field. If Fe snow can explain the observed early magnetic field, it could explain the simultaneous absence of a present-day magnetic field and presence of a potential present-day inner core. The existence of the latter is planned to be probed by the NASA Insight mission [10].

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TOWARDS A NEW TOOL FOR MODELLING NON-ADIABATIC GIANT PLANETS

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We present work in progress towards a modelling approach for the interior and evolution of giant planets. It follows the well-known method by Henyey et al. (1964) [1] for stars.
In contrast to conventional modelling assumptions for Jupiter and Saturn [2] and Uranus and Neptune [3], our goal is to go beyond the premise of adiabatic interiors, as the presence of stably stratified and thus non-adiabatic regions is indicated by some magnetic field models for the ice giants [4]. Therefore, we solve self-consistently for the local temperature gradient, the compositional gradient and the heat flux, accounting for heat and particle transport by convection and diffusion. This way we hope to gain new insight into the origin of the low intrinsic luminosity of Uranus and the high intrinsic luminosity of Neptune. Here, we present the theoretical foundations and implementation of the model as well as first results.

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STRUCTURE OF SiO_2 MELTS AT ULTRAHIGH PRESSURES – THE EXPERIMENTAL AND AB INITIO APPROACH

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SiO_2 is one of the most fundamental constituents in planetary science, being vastly abundant in the Earth's crust and mantle. As an essential 'building block', it bonds with Mg, Fe and other elements to form major mineral phases and even free SiO_2 can be expected in localized regions in the Earth's mantle, derived from e.g. subducted oceanic crust [1]. The stability of SiO_2 within these regions is affected by polymorphism at high pressures and SiO_2 serves as an archetype for the dense highly coordinated silicates of planetary interiors and large ($1- 10M_\oplus$) exoplanets [2]. Seismological heterogeneities in the ultralow velocity zones (ULVZs) at the upper end of the transition zone and at the core mantle boundary (CMB) have been interpreted with the presence of higher coordinated SiO_2 melts [3, 4]. The possible presence of silicate melts may result from partial melting of the lowermost mantle minerals or are remnants of the dense basal magma ocean [5], however, up to date it is only little known about these SiO_2 melts within the field of geosciences. Recent studies on SiO_2 glass with the use of diamond anvil cells at ambient temperatures indicate a change in coordination from 4– to 6–fold up to pressures of 50 GPa and from 6– to 6.8– fold in the pressure range of 50 to 172 GPa [6]. With the use of X– probe ray free SiO_2–electron lasers to its liquidus regime and obtain information about SiO_2 (XFELs) and high energy–, long pulse optical lasers, we will be able to melt structures on the lattice level. Simultaneous {ab initio} molecular dynamic (AIMD) calculations and X–ray diffraction simulations will be done along the SiO_2 – Hugoniot up to its melting regime with emphasis on Si– melts. O bond length and coordination. Here we present an experimental set up at X – ray free –electron lasers and preliminary AIMD results on the structural properties of SiO_2.

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P-V-T EQUATION-OF-STATE OF LIQUID FE FROM AB-INITIO SIMULATIONS TO THE TPA REGIME

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The pressure-volume-temperature (P-V-T) equation-of-state (EoS) of liquid iron provides important information (reference adiabat, density ρ and higher order thermodynamic parameters) in the modelling of the internal structure of planetary bodies with Fe-based cores. Relevant P-conditions range from a few GPa (Moon, Mercury) through the Mbar range (Earth) to several TPa (super-Earth exoplanets). Experimental data on ρ in the liquid stability field are scarce and a thermodynamic assessment of ρ depends on matching Gibbs energy along the melting line which remains controversial to this day. The alternative determination of a P-V-T EoS based on ab-initio simulations, on the other hand, suffer from the fact that ρ at ambient P is predicted too large by as much as 20% in the simulations [e.g., 1]. Here, we have fitted P-V-T triplets from ab-initio molecular dynamics simulations with an EoS formulation that is thermodynamically self-consistent [2] and combined it with a correction formalism that accounts for the known ρ-mismatch at ambient P [3]. As the correction is additive to the Helmholtz potential and shows the correct limiting behavior at high and low ρ, the thermodynamic self-consistency of the results is not affected. Using this combination, the EoS we have developed reproduces ρ from shock-wave experiments as well as previous models, but shows a significantly improved agreement at ambient P, the critical point and the sole low ρ measurement at 4.3 GPa.

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FROM Tram station: **S-Bahnhof Adlershof**

Departure Times:

Tram **63**: 18:11, 18:31, 18:51, …
Tram **61**: 18:04, 18:24, 18:44, …

Travel Time: 10 minutes

Ticket-vending machine inside Tram: 1,70 € (single ticket "Kurzstrecke")

For the return ride, please use Tram **63** or **61** (direction Adlershof, Karl-Ziegler-Str.)
or Tram **60** (direction S-Bahnhof Adlershof).

Return FROM Tram station: **Rathaus Köpenick** (opposite to Ratskeller Köpenick)

Departure Times:

Tram **63**: …, 21:45, 22:05, 22:25, …, 00:05.
Tram **61**: …, 21:55, 22:15, 22:35.
Tram **60**: 00:22, 00:37, 00:42, 00:57, 01:02.

Travel Time: 10 minutes

Ticket-vending machine inside Tram: 1,70 € (single ticket "Kurzstrecke")

We look forward to meeting you at the

8th Joint Workshop on High Pressure, Planetary, and Plasma Physics
October 9 - 11, 2019
Helmholtz Zentrum Dresden-Rossendorf (HZDR), Germany

- Evolution and structure of giant planet interiors,

- Interior structure, bulk composition, and internal geodynamics of solid planets,

- Deep volatile cycles and exchange processes between geochemical reservoirs,

- Physics and chemistry of impact processes,

- Equations of state, petrology, and geochemistry of planetary materials,

- Melting relations and phase transformations of materials at extreme states,

- Dynamic and ultrafast processes in strongly excited solids or similar,

- Laboratory experiments using multi-anvil and diamond-anvil cells,

- Ab initio simulation studies for matter under extreme conditions.