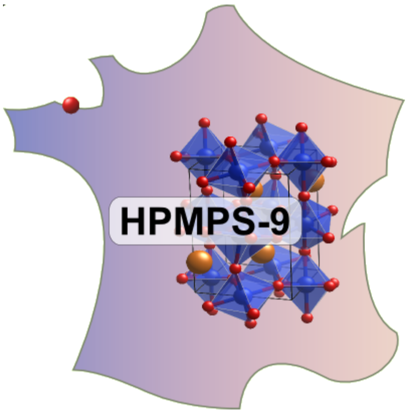
Palais du Grand Large, Saint Malo, France
September 24-28, 2017



9th High Pressure Mineral Physics Seminar

Program and abstracts

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With many thanks to **Hortense Apan** and **Nalini Loret**

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Conference Program

High Pressure Mineral Physics Seminar

24-28 Sep 2017 – Saint Malo (France)

Program Outline

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08:00					
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		Keynote lecture by J.-P. Poirier			
09:00			Oral session	Oral session	Oral session
		Oral session			
10:00					
		Coffee and poster session	Coffee and poster session	Coffee and poster session	Coffee
11:00					Oral session
		Oral session	Oral session	Oral session	
12:00					
		Lunch in conference center	Lunch in conference center	Lunch in conference center	Lunch in conference center
13:00					
14:00		Keynote lecture by T. Tsuchiya	Keynote lecture by B. Buffett	Keynote lecture by D. Andrault	
		Oral session	Oral session	Oral session	
15:00					
16:00					
		Coffee and poster session	Coffee and poster session	Coffee and poster session	
17:00	Ice breaker and welcome reception				
		Oral session	Oral session	Oral session	
18:00					
19:00				Conference dinner	
		Dinner in conference center			
20:00					
21:00					
22:00					

Monday, September 25, 2017

8:30 - 8:50	Welcome session
8:50 - 9:20	Keynote lecture by *Jean-Paul Poirier* : 40 years of High-pressure Mineral Physics
9:20 - 10:20	HPMPS-11
09:20 - 09:40	› Supercritical silicate melts in the protolunar disk - *Caracas Razvan* (invited)
09:40 - 10:00	› Properties of deep mantle melts - *Chrystele Sanloup*
10:00 - 10:20	› Constraining Earth's composition, mineralogy and its heat production - *William McDonough* (invited)
10:20 - 11:30	Coffee and poster session
11:30 - 12:30	HPMPS-12
11:30 - 11:50	› Budget of radioactive elements (K, U) in Bulk Earth - *Ingrid Blanchard*
11:50 - 12:10	› East-west mantle geochemical hemispheres and their implications for top-down hemispherical dynamics - *Hikaru Iwamori* (invited)
12:10 - 12:30	› Seismic anisotropy tomography and mantle dynamics - *Dapeng Zhao* (invited)
12:30 - 14:00	Lunch in conference center
14:00 - 14:30	Keynote lecture by *Taku Tsuchiya*: Theory and Computation for High-Pressure Mineral Physics
14:30 - 16:10	HPMPS-13
14:30 - 14:50	› Structure-elastic behaviour relationship in minerals at high-pressure - *Tiziana Boffa Ballaran* (invited)
14:50 - 15:10	› On pure climb creep mechanism in the lower mantle - *Philippe Carrez* (invited)
15:10 - 15:30	› Grain boundary diffusion of W and Re in lower mantle phases - *Takashi Yoshino* (invited)
15:30 - 15:50	› Affect of pressure on MgO grain boundary migration; Implications for grain growth. - *Jac van Driel*
15:50 - 16:10	› Effect of water on the rheology of clinopyroxene at high temperature and pressure - *Junfeng Zhang*
16:10 - 17:30	Coffee and poster session
17:30 - 18:50	HPMPS-14
17:30 - 17:50	› Some recent developments in electron microscopy analysis of samples recovered from high pressure experiments - *Hiroaki Ohfuji* (invited)
17:50 - 18:10	› Seismic Anisotropy of the D″ Layer induced by (001) Deformation of Post-Perovskite - *xiang wu*
18:10 - 18:30	› Electron channeling contrast imaging of individual dislocations in geological materials using a field emission scanning electron microscope - *Nobuyoshi Miyajima*
18:30 - 18:50	› Synthesis of transparent nano-ceramics at high pressure and temperature - *Tetsuo Irifune*
19 :30 - 22:00	Dinner in conference center

Tuesday, September 26, 2017

8:30 - 9:00	Keynote lecture by *Yigang Xu*: Linking the earth interior processes and surface system evolution: A CAS priority strategic program
9:00 - 10:20	HPMPS-21
09:00 - 09:20	› Experimentally determined grain growth kinetics of the spinel structure through the upper mantle to 660 km - *Isra Ezad*
09:20 - 09:40	› Study Of Perovskite / Post-Perovskite Phase Transformation Mechanism By Using Multigrain Crystallography - *Christopher Langrand*
09:40 - 10:00	› The interaction between deformation and the olivine-spinel transformation in fayalite - *Tomoaki Kubo* (invited)
10:00 - 10:20	› The Mantle Transition Zone history of Tibetan chromitites: experimental constraints - *Yanfei zhang*
10:20 - 11:30	Coffee and poster session
11:30 - 12:30	HPMPS-22
11:30 - 11:50	› Core-Mantle Interactions: Past and Present - *James Badro* (invited)
11:50 - 12:10	› Light element diffusion in liquid Fe for P-T conditions of the Earth's interior - *Gerd Steinle-Neumann*
12:10 - 12:30	› Electrical conductivity of silicate liquids at extreme conditions and planetary dynamos - *Lars Stixrude*
12:30 - 14:00	Lunch in conference center
14:00 - 14:30	Keynote lecture by *Bruce Buffett*: Chemical Exchange between Earth's Core and Mantle
14:30 - 16:10	HPMPS-23
14:30 - 14:50	› Phase transition boundary between fcc and hcp structures in the system Fe-Si and its implications for thermodynamics of silicon-bearing Earth's core - *Tetsuya Komabayashi* (invited)
14:50 - 15:10	› Triple point hcp-fcc-liquid in pure Fe phase diagram determined by in-situ XANES diagnostic - *Guillaume Morard*
15:10 - 15:30	› Thermoelastic properties of hcp-Fe-Si-C-S alloys under the Earth's inner core conditions - *Yunguo Li*
15:30 - 15:50	› High-pressure equation of state of Fe-rich liquids and the solidification of molten planetary cores - *Zhicheng Jing* (invited)
15:50 - 16:10	› Nuclear resonant x-ray scattering studies under high pressure: The case for 57Fe, 119Sn, 151Eu, and 161Dy metal and their compounds - *Esen Ercan Alp*
16:10 - 17:30	Coffee and poster session
17:30 - 18:30	HPMPS-24
17:30 - 17:50	› Sound velocity of iron-light element compounds and composition of the inner core - *Eiji Ohtani*
17:50 - 18:10	› Sound velocity and elastic properties of liquid Fe–Ni–Si at high pressure - *Hidenori Terasaki*
18:10 - 18:30	› Formation of non-stoichiometric fcc and hcp FeHx at high pressure and temperature conditions - *Shoh Tagawa*
19:00 - 23:30	Free evening - Enjoy Saint Malo city !

Wednesday, September 27, 2017

8:30 - 9:00	Keynote lecture by *Carmen Sanchez-Valle*: Fluids geochemistry at extreme conditions in subduction zones
9:00 - 10:20	HPMPS-31
09:00 - 09:20	› High-pressure phase transitions in AlOOH and FeOOH - *Masayuki Nishi* (invited)
09:20 - 09:40	› Coupling deformation under high pressures, synchrotron X-rays and acoustic emissions monitoring for the study of deep earthquakes - *Nadège Hilairet* (invited)
09:40 - 10:00	› Water and carbon cycle in global-scale mantle dynamics modeling - *Takashi Nakagawa* (invited)
10:00 - 10:20	› Immiscible Hydrocarbon Fluids in the Mantle - *Isabelle Daniel*
10:20 - 11:30	Coffee and poster session
11:30 - 12:30	HPMPS-32
11:30 - 11:50	› The effect of hydration on the elastic properties of ringwoodite at transition zone pressures - *Kirsten Schulze*
11:50 - 12:10	› Experimental study on the stability of methane hydrate under high pressure and high temperature - *Hirokazu Kadobayashi*
12:10 - 12:30	› Exploring new phenomena in salty ices and ice clathrates under planetary conditions - *Livia Bove*
12:30 - 14:00	Lunch in conference center
14:00 - 14:30	Keynote lecture by *Denis Andrault*: Melting properties of the deep Earth's mantle: Implications for the magma ocean crystallization
14:30 - 16:10	HPMPS-33
14:30 - 14:50	› Eutectic melting in the MgO-SiO2 system and its implication to Earth's lower mantle evolution - *Marzena Baron* (invited)
14:50 - 15:10	› The High-Pressure Structure of Silicate Melts and the Impact on Magma Ocean Evolution - *Aaron Wolf* (invited)
15:10 - 15:30	› Structure of silicate glasses up to 172 GPa - *Clemens Prescher* (invited)
15:30 - 15:50	› Density and structure of amorphous silicates at high pressure conditions - *Sylvain Petitgirard*
15:50 - 16:10	› Densification mechanisms of amorphous silicates at high pressure and temperature - *Alisha Clark*
16:10 - 17:30	Coffee and poster session
17:30 - 18:30	HPMPS-34
17:30 - 17:50	› Experimental evidence supporting global melt layer at the base of the Earth's upper mantle - *Geeth Manthilake* (invited)
17:50 - 18:10	› Computational and experimental studies of iron-bearing carbonates and silicate glasses at lower mantle pressures - *Natalia Solomatova* (invited)
18:10 - 18:30	› High Speed X-ray imaging for studying behavior of liquids at high pressures and high temperatures - *Eglantine Boulard* (invited)
19:00 - 23:00	Conference dinner in Saint Malo's harbour onboard "Etoile du Roy"

Thursday, September 28, 2017

8:30 - 9:00	Keynote lecture by *Thomas Duffy*: Dynamic Compression: From Meteorites to Exoplanets
9:00 - 10:20	HPMPS-41
09:00 - 09:20	› Picosecond Acoustics : a way to Thermodynamical Properties of Solids and Liquids at Extreme Conditions - *Simon Ayrinhac* (invited)
09:20 - 09:40	› Development of ultrasonic measurement technique under lower mantle conditions - *Yuji Higo* (invited)
09:40 - 10:00	› High-pressure single-crystal elasticity measurements of Al-Fe-bridgmanite up to lower mantle pressures - *Hauke Marquardt* (invited)
10:00 - 10:20	› Crystal structure of MgO along the shock Hugoniot - *June Wicks* (invited)
10:20 – 11:00	Coffee break
11:00 - 12:00	HPMPS-42
11:00 - 11:20	› Perspectives for static and dynamic high-pressure experiments at the High Energy Density Science (HED) instrument at European XFEL - *Karen Appel* (invited)
11:20 - 11:40	› Amorphous and liquid samples structure and density measurements at high pressure – high temperature using diffraction and imaging techniques - *Nicolas Guignot*
11:40 - 12:00	› MSPD beamline for high pressure studies at Alba synchrotron - *Catalin Popescu*
12:00 - 12:30	Awards and closing ceremony
12:30 - 14:00	Lunch in conference center

Keynote lectures

Melting properties of the deep Earth's mantle: Implications for the magma ocean crystallization

Denis Andrault * [1]

[1] Laboratoire Magmas et Volcans (LMV) – Université Clermont Auvergne, CNRS – Campus Universitaire des Cézeaux, 6 Avenue Blaise Pascal, 63178 AUBIERE, France

A large proportion of our planet experienced melting in the course of its accretion history as a consequence of the energy release associated with large impacts, radioactive decay and core formation. Major unknowns remain about this early time, for example the extension depth of the magma ocean and the chemical signature inherited from the mantle crystallization. For this reason, we must refine the melting properties of the primitive mantle, in order to address the possible occurrence of chemical heterogeneities between distinct geochemical reservoirs.
In the past 5-10 years, several experimental works tentatively addressed the melting properties of different types of materials relevant to the deep mantle. Almost all studies used the laser heated diamond anvil cell, which can now routinely generate P-T conditions up to more than 135 GPa and 6000 K. Unfortunately, temperature gradients are unavoidable, especially the axial gradient between the two diamonds, which makes the interpretation of experimental results more challenging. Still, synchrotron-based X-ray diffraction was broadly used to determine the onset of melting and the sequence of phase disappearance, while several complementary *in situ* (XANES, XRF, etc.) and *ex situ* (FIB, SEM, EPMA, ...) techniques have considerably strengthened our knowledge about melting properties at lower mantle conditions.

In this presentation, some recent technical improvements and major scientific findings will be reviewed. Geophysical implications will tentatively address these specific questions:

- Did a basal magma ocean appeared in the lowermost mantle after the moon forming impact?

- Should we expect mantle overturns at the end of the magma ocean crystallization?
- Is the current D"-layer likely correlated, or not, with the early magma ocean crystallization?

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*Speaker

Chemical Exchange between Earth's Core and Mantle

Bruce Buffett * [1]

[1] Bruce Buffett (UC Berkeley) – 307 McCone Hall, Berkeley, CA 94720-4767, United States

Transfer of mass across the core-mantle boundary (CMB) is a consequence of chemical disequilibrium. Initial departures from equilibrium are established by the process of core formation during the accretion of the planet. Measured concentrations of moderately siderophile elements in the mantle are compatible with separation of metal and silicates at the bottom of a mid-mantle magma ocean (P 50 GPa and T 3300 K). Subsequent delivery of liquid metal to the core is thought to occur in large diapirs with limited chemical exchange. This material arrives at the CMB well out of equilibrium with the surrounding mantle. Adjustments toward equilibrium are expected to drive Si and/or O from the mantle into the core. The rates of mass flux are initially limited by chemical diffusion through the core, but solid-state diffusion through the mantle quickly becomes the rate-limiting process. Small amounts of partial melt can lower this barrier, so quantitative estimates for the delivery of light element to the core depend on the longevity of partial melt at the base of the mantle. Diffusion of Si or O into the core is capable of producing a 60-km to 120-km stratified layer over the age of the Earth, independent of how mass is transferred to the core. By comparison, estimates for the strength of the density stratification are sensitive to factors such as degree of partial melt in the mantle. Gradual cooling of the core shifts the state of chemical equilibrium with the mantle and may cause other dissolved constituents (like Mg) to become oversaturated. Exsolution of Mg promotes compositional convection in the core and tends to erase any stratification. We distinguish between these possibilities at the present time by looking for the influence of fluid stratification on flow at the top of the core. Recent evidence for magnetic waves in the core supports the existence of a 140-km stratified layer. The strength of stratification is broadly consistent with a thermal origin, although a compositional origin is also possible if transport into the core is limited by small volumes of partial melt in the mantle. In order to explain the thickness of the layer with compositional gradients, we favor O as the main additive to the core after its initial formation.

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[*] Speaker

Dynamic Compression: From Meteorites to Exoplanets

Thomas Duffy * [1]

[1] Princeton University – Department of Geosciences, United States

Dynamic compression studies have applications to problems in Earth and planetary science ranging from understanding the effects of impacts and explosions to the synthesis of new high-pressure phases of the deep Earth. In this talk I will describe two major new advances in this area. Laser-based dynamic compression provides opportunities to study the structures and properties of geological materials to ultrahigh pressure conditions reaching 1 terapascal and beyond. By controlling the shape and duration of the incident laser pulse, either shock or ramp (shockless) loading can be produced. By combining these techniques with pulsed x-ray diffraction, we have explored a variety of materials including iron silicide, magnesium oxide, and carbon to ultrahigh pressures relevant to exoplanet interior conditions. A second major new development is the Dynamic Compression Sector at the Advanced Photon Source which provides the capability to couple gas-gun shock-wave experiments with brilliant synchrotron X-rays. Here I will show results on the lattice-level structural response of quartz and fused silica under shock loading that provide a new understanding of the behavior of silicate minerals under dynamic compression.

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*Speaker

40 years of High-pressure Mineral Physics

Jean Paul Poirier *† 1

1 Institut de Physique du Globe de Paris - Université Sorbonne Paris Cité (IPGP) – Institut de Physique du Globe de Paris, Université Sorbonne Paris Cité – 1 Rue Jussieu 75005 Paris, France

The introductory talk will focus on the considerable advances, both experimental and computational, in High-pressure Mineral Physics in the last forty years and the ensuing better understanding of the structure and workings of the inner Earth.

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[*] Speaker

[†] Corresponding author: poirier@ipgp.fr

Fluids geochemistry at extreme conditions in subduction zones

Carmen Sanchez-Valle *† [1], Alexandra Tsay [2], Zoltan Zajacz [2], Marion Louvel [3], Daniel Grolimund [4], Denis Testemale [5]

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[2] Department of Earth Sciences, University of Toronto – 22 Russell St., M5S 3B1, Toronto, Canada
[3] School of Earth Sciences, University of Bristol – Queens Road, Bristol BS81RJ, United Kingdom
[4] Swiss Light Source, Paul Scherrer Institute – 5232 Villigen PSI, Switzerland
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High pressure slab-derived fluids (aqueous fluid, hydrous melt or supercritical fluid?) are major vectors for mass transfer and element recycling in subduction zones. The quantitative estimates of mass recycling the Earth's interior are, however, limited by the poor understanding of the atomic-scale mechanims that control the mobilization and transport of elements during fluid-rock interactions in deep settings. In the last decade, new experimental designs combining high-pressure vessels and advanced micro-analytical techniques have opened the possibility for monitoring *in situ* the chemical composition, the molecular-scale structure and thermodynamic quantities for high-pressure fluids. Here, we will discuss emerging views on the mechanism of mobilization and recycling of trace elements and the nature and redox state of the slab flux in the light of hydrothermal experiments based on synchrotron techniques and the analysis of fluids trapped in synthetic fluid inclusions (SFI) at high pressure. Specifically, we will present results on the speciation, solubility and partition of trace and redox sensitive elements (e.g, REE, HFSE, Fe) in the eclogite-fluid system that illustrate the key role of coordination chemistry in the recycling of elements upon slab dehydration. The picture that is emerging from these studies is that ligand-bearing aqueous phases may have comparable efficiency to hydrous silicate melts in the mobilization and fractionation of trace elements, and that their role as mass transfer agents in subduction-related processes may have been underestimated until now. Finally, we will provide estimates of element fluxes and the oxidizing capacity of fluids released upon slab dehydration in the shallow upper mantle and discuss the implication for the geochemical signature of arc magmas.

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[*] Speaker

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Theory and Computation for High-Pressure Mineral Physics

Taku Tsuchiya *† [1,2], Jun Tsuchiya [1], Haruhiko Dekura [1], Zhihua Xiong [1],
Sebastian Ritterbex [1], Xianlong Wang [3], Hiroki Ichikawa [2]

[1] Geodynamics Research Center, Ehime University (GRC, Ehime Univ.) – Japan
[2] Earth-Life Science Institute, Tokyo Institute of Technology (ELSI, Tokyo Tech.) – Japan
[3] Chinese Academy of Sciences – China

Recent progress in theoretical mineral physics (TMP) based on the density functional quantum mechanical theory has been dramatic in conjunction with the advancement of computer technologies. It is now possible to predict high-P,T equation of state and phase stability of complex minerals quantitatively with uncertainties that are comparable to or even smaller than those attached in experimental data. The technique is now routinely applied not only for theoretical backup to experiments but also for guide to experiments [1]. Our next grand challenges include new technical developments for high-P,T thermophysical and thermochemical properties, such as thermoelasticity [2], thermal conductivity [3], elemental diffusivity [4], chemical partitioning of both solid and liquid phases [5] within the correlated systems. Thermoelasticity and thermal conductivity, which are calculated based on the harmonic and anharmonic lattice dynamics theories, are keys to clarifying compositional and thermal properties of the deep mantle and core through interpreting seismological information, respectively. Chemical partitioning, which we can access using the thermodynamic integration method, on the other hand allows us to link mineral physics to geochemistry. In this talk I will report recent activities in the Ehime Univ. TMP group. References:

[1] M. Nishi, Y. Kuwayama, J. Tsuchiya, T. Tsuchiya, Nature 547, 205 (2017)
[2] X. Wang, T. Tsuchiya, A. Hase, Nature Geo. 8, 556 (2015).
[3] H. Dekura, T. Tsuchiya, Phys. Rev. B 95, 184303 (2017).
[4] S. Ritterbex, T. Harada, T. Tsuchiya, under rev.
[5] Z. Xiong, T. Tsuchiya, T. Taniuchi, in prep.

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[*] Speaker

[†] Corresponding author: tsuchiya.taku.mg@ehime-u.ac.jp

Linking the earth interior processes and surface system evolution: A CAS priority strategic program

Yigang Xu * [1]

[1] Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, 510640 Guangzhou, China – China

It is well known that earth's interior is the principle engine of the operation of our planet. However, how to link the earth's interior processes and surface system evolution remain challenged. The recent launched Priority Strategic Program of Chinese Academy of Sciences (CAS) focuses on this subject by bringing together experts of different disciplines ranging from seismology, experimental petrology, geochemistry, geodynamical modeling, plaeo-environment reconstruction and paleopentology. The project comprises three mutually related topics: (1) composition and structure of main boundaries of the earth's interior; (2) interaction between earth's interior layers and material recycling; and (3) surface responses to deep earth processes. This talk briefly introduces some of key scientific questions that this project addressed and highlights some relevant progresses.

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*Speaker

Monday, morning

Constraining Earth's composition, mineralogy and its heat production

William Mcdonough * [1,2,3]

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[3] Tohoku University – 6-3 Aramaki-aza-Aoba Aoba-ka, Sendai 980-8578, Japan

Geoneutrinos, produced during beta decays of naturally occurring radioactive isotopes in the Earth, are a unique direct probe of our planet's interior. The kTon-scale, underground, liquid scintillation detectors in Japan and Italy, which measure the flux of these electron antineutrinos, reveal that radiogenic heat from the decay of Th and U (only detectable signal) contributes between 20% and 50% of the Earth's present-day power (46+/-3 TW). Geoneutrino studies are providing quantitative constraints of the amount of uranium and thorium inside the Earth. Knowing precisely the absolute U and Th content of the Earth defines the planet's nuclear power budget for the heat producing elements. It also explicitly defines the absolute abundances of the refractory elements in the planet, which in turn specifies the mode proportion of Ca-pervoskite in the lower mantle. I will report on the latest data from geoenutrino studies and the data expected to be obtained over the next 8 years. These data will critically evaluate competing models of the bulk silicate Earth (i.e., low, medium, and high Q models, respectively, 10, 20, and 30 ppb U, Th/U = 4, and K/U =1.4x10ˆ4) and exclude some at the 1-sigma level. By 2025 there are projected to be 5 detectors counting the Earth's flux of geoneutrinos (10ˆ25/s); each will define locally the radiogenic power in the immediate (500 km) crust and collectively, the global array of detectors will define the residual radiogenic power left in the mantle and the Earth's Th/U value. Ongoing studies presently reveal that the Earth's Th/U value is 3.9 +/-0.15, a value coincident with that of the solar system. Consequently, given the marked differences in the partitioning behavior of Th and U between metal and silicate, this well constrained Th/U value for the bulk silicate Earth documents that negligible Th and U is in the core. Geoneutrino studies provide critical constraints on the power driving plate tectonics, mantle convection, and the geodynamo.

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*Speaker

Supercritical silicate melts in the protolunar disk

Caracas Razvan * [1]

[1] CNRS, ENS de Lyon, Laboratoire de Geologie de Lyon (LGL) – CNRS : UMR5276 – CNRS, ENS Lyon, Laboratory of Geology of Lyon, France

We employ large-scale molecular dynamics simulations to understand the physical and chemical behaviour of the magma ocean during the Giant Impact. We use the density-functional theory to compute the forces under which the atoms move according to Newtonian mechanics. For this we employ the VASP implementation.
Under pressure we find an increase of the coordination number of all atomic species, as a mechanism for accommodating compression, and a linear decrease of the self-diffusion. Iron atoms exhibit a gradual reduction of their magnetic moment.

We identify the supercritical region characterized by one homogeneous fluid, rich in ionic species. We show that the chemical speciation is very different from the one obtained at ambient pressure conditions. At lower temperatures, in the 2000 – 4000 K, we capture the nucleation of bubbles. When volatiles are present in the system, such molecular species, they are the first ones to evaporate and be present in these bubbles. We propose numerical tools to detect the liquid-vapor equilibrium. This is reached consistently regardless of the thermodynamic path.
Acknowledgements: This research was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement n○681818 – IMPACT). The ab initio simulations were performed on the GENCI supercomputers, under eDARI/CINES grants x106368.

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*Speaker

Properties of deep mantle melts

Chrystele Sanloup * [1]

[1] Universite Pierre et Marie Curie (UPMC) – Université Pierre et Marie Curie (UPMC) - Paris VI, Université Pierre et Marie Curie [UPMC] - Paris VI – France

Magmas in the current day Earth are produced essentially at lithospheric pressures, at the exception of ultra deep melts detected by seismology at the mantle-core boundary. The latter are possible remnants of the early magma ocean or result from partial melting of rocks with a lower melting point than the bulk mantle. Exploring the physical properties of magmas at such depths is therefore key to understanding the nature and origin of these melts. It is now possible to collect in situ synchrotron X-ray diffraction data collected on deep mantle melts up to the megabar range, and extract some quantitative information on interatomic distances and density. Data collected on molten basalt and molten carbonate using laser-heated diamond anvil cells will be presented, along with complementary X-ray Raman data collected on quenched carbonate samples. The structural information on both type of melts will be discussed, along with the implications for their likely contrasting mobility at depth.

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*Speaker

Budget of radioactive elements (K, U) in Bulk Earth

Ingrid Blanchard * [1,2], Julien Siebert [1], James Badro [1]

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The inner dynamics of the Earth is intimately linked to the energy budget of the planet. Several sources contribute to the heat budget such as the primordial heat or the latent heat linked to the crystallization of the inner core. Another substantial source is the radioactive decay of long lived radionuclides (K, U and Th). To accurately describe the heat engine that is the planet, one has to infer the composition of the core in terms of these radioactive elements. Presence of potassium in the core has been suggested in the early 70's, and has been the subject of numerous metal-silicate partitioning studies at various conditions of pressure and temperature using large volume presses. In another hand, uranium solubility in liquid iron has been shown to increase with high temperature and sulfur content of the metal.

Here, we conducted metal-silicate partitioning study of potassium and uranium using the laser-heated diamond anvil cell technique to investigate P-T conditions directly relevant to core-mantle equilibration at the base of a deep magma ocean. We have tested the effects of pressure, temperature, but also silicate and metal composition with starting material that were either basaltic or pyrolitic and with or without sulfur. We show that high pressures enhance potassium solubility in the metal, whereas uranium is more sensitive to the presence of oxygen in the core and to high temperatures. Sulfur has no effect on potassium and uranium metal silicate partitioning at the condition of our experiments.
Our results have ultimately been incorporated in continuous core formation models to calculate the amount of potassium and uranium that can be expected in the Earth's core and thus, estimate the Bulk Earth composition of these radionuclides.

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*Speaker

East-west mantle geochemical hemispheres and their implications for top-down hemispherical dynamics

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Global geochemical structures of the mantle have been statistically investigated in both spatial and compositional domains, using a total of 6854 young basalt data consisting of five isotopic ratios of Sr, Nd and Pb from almost all tectonic settings (mid-ocean ridge, ocean island, arc and continent). Characteristic features hidden in the data have been extracted using multivariate analysis "Independent Component Analysis" and "Whitening K-means Cluster Analysis" (Iwamori and Nakamura, 2015, Gondwana Res.; Iwamori et al., 2017, G-cubed). Two independent components (IC1 and IC2) explain most of the sample variance (95%), and the third minor component (IC3) accounts for 4%. Therefore, almost all young basalts covering the whole globe plot on a single compositional plane, and can be explained by only two differentiation processes (i.e., melting and aqueous fluid-rock interaction). IC1 represents 'anciently subducted melt component' stored for 0.8 to 2.4 Gyr in the mantle, and positive IC1 characterizes the hotspots except for Hawaii and Iceland. IC2 represents 'anciently subducted aqueous fluid component' stored for 0.3 to 0.9 Gyr in the mantle, and defines the fluid component-rich (=positive IC2) eastern hemisphere. We have also found a striking geometrical similarity between the IC2 and the inner core hemispheric structures: the eastern hemisphere shows positive IC2 in the mantle and high seismic velocities in the inner core. Combining these constraints, we propose 'top-down hemispherical dynamics' (Iwamori and Nakamura, 2015, Gondwana Res.): focused subduction within and around the supercontinent has created a fluid component-rich hemisphere with a lower temperature, compared to the oceanic mantle. The colder hemisphere seems to have been anchored to the asthenosphere during the continental dispersal, and may affect the temperature and growth rate of the inner core, resulting in the coupled hemispherical structures in the mantle and the core.

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*Speaker

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Seismic anisotropy tomography and mantle dynamics

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Seismic anisotropy tomography is a new but powerful tool for mapping 3-D variations of seismic anisotropy in the crust and mantle, shedding new light on mantle flow and subduction dynamics (e.g., *Zhao et al.*, 2016; *Liu and Zhao*, 2017). We determined 3-D P-wave anisotropic tomography of the NW Pacific subduction zones (*Wei et al.*, 2015), which show that the intraplate volcanism is caused by hot and wet upwelling in the big mantle wedge above the stagnant Pacific slab. The fast velocity direction (FVD) in the subducting Philippine Sea slab beneath the Ryukyu arc is trench parallel, being consistent with the spreading direction of the West Philippine Basin during its initial opening stage, which may reflect the fossil anisotropy. A striking variation of the FVD with depth is revealed in the subducting Pacific slab beneath the Tohoku arc, which may be caused by slab dehydration that changed elastic properties of the slab with depth. The FVD in the mantle wedge beneath the Tohoku and Ryukyu arcs is trench normal, reflecting subduction-induced convection. Beneath the Kuril and Izu-Bonin arcs, the FVD in the mantle wedge is nearly normal to the moving direction of the downgoing Pacific plate, suggesting that the oblique subduction together with the complex slab morphology have disturbed the mantle flow. We also determined 3-D Vp anisotropic tomography in the mantle beneath SE Asia, which shows the high-velocity (high-V) subducting slabs clearly in the upper mantle and the MTZ. Low-velocity (low-V) zones with trench-normal anisotropy are revealed in the uppermost mantle, which indicate back-arc spreading or secondary mantle-wedge flow induced by the slab subduction. In contrast, trench-parallel anisotropy dominates in the deep upper mantle and reflects structures either in the subducting slab or in the upper mantle surrounding the slab. A low-V body extending down to the lower mantle is visible under the Hainan volcano far away from the plate boundaries, suggesting that Hainan is a hotspot fed by a lower-mantle plume. The low-V body under Hainan is connected with low-V zones in the upper mantle under SE Tibet and Vietnam.

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[*] Speaker
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Monday, afternoon

Structure-elastic behaviour relationship in minerals at high-pressure

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Since the first pioneer studies in the 1970s on the high-pressure behavior of single-crystal materials conducted with a diamond anvil cell using X-ray diffraction, continuous developments of cell design and instrumentation has given rise to an exponential increase of publications in a wide range of scientific disciplines including Earth and material sciences, chemistry, physics, biology etc. In Earth Sciences in particular, single-crystal X-ray diffraction has been used a powerful tool in several studies for the following reasons: 1) it allows determining the compressibility of different minerals in order to provide important constraint for thermodynamic models of the Earth's interior; 2) it allows the structural characterization of new high-pressure phases; 3) it gives insight on the structural variations of mineral as a function of composition, pressure and temperature and thus the influence that such changes have on their elastic properties. In this contribution we will use bridgmanite, the MgSiO3 perovskite-type structure, as an example to show how single-crystal X-ray diffraction data collected at room and high-pressure can be used to pinpoint the structural changes associated with Al and Fe substitution in the MgSiO3 end-member structure and how such changes influence the high-pressure behaviour of bridgmanite at the conditions of the Earth's lower mantle, providing important constrain on seismic models.

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*Speaker

On pure climb creep mechanism in the lower mantle

Philippe Carrez * [1], Francesca Boioli [1], Patrick Cordier [1], Benoit Devincre [2], Karine Gouriet [1], Pierre Hirel [1], Antoine Kraych [1]

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It is usually assumed that diffusion creep is the main deformation mechanism in the lower mantle. However, this puts quite strong constraints on grain sizes and point defect concentrations. Along this line, several experimental or theoretical studies have recently highlighted the fact that high lattice friction is opposed to dislocation glide in silicates from the deep mantle under pressure, especially in bridgmanite. In this presentation, we further investigate this aspect by providing quantitative estimates for dislocation mobilities in both glide and climb from atomic scale modelling. We show that under low stress conditions representative of the mantle, dislocation creep operates under conditions very different from those activated at laboratory strain-rates. We propose that the creep in the deep mantle can result from pure dislocation climb processes. Based on dislocation dynamics models, we show that pure climb creep is an efficient strain-producing mechanism in bridgmanite in the conditions of the lower mantle, which is grain size insensitive. Involving pure climb of dislocations with no shear, this creep mechanism is compatible with the absence of seismic anisotropy in the Earth's lower mantle.

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*Speaker

Grain boundary diffusion of W and Re in lower mantle phases

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Tungsten and rhenium grain boundary diffusion coefficients in the lower mantle phases was determined at 25 GPa and temperatures ranging from 1,873 to 2,173 K using a Kawai-type multianvil press. Because grain-boundary concentrations are expected to be very low, multi-sink method was used to determine the diffusion profile. Pt particles with a size of 10 to 20 μm were used as sinking material for siderophile elements. High-pressure diffusion experiments were performed on pre-synthesized polycrystalline postspinel and bridgmanite with scattered Pt sink particles sandwiched by W and Re foils. Recovered samples were sectioned perpendicular to the diffusion interface and W and Re concentrations in Pt sink particles were examined by an electron microprobe and a laser ablation multi-collector inductively coupled plasma mass spectroscopy (LA ICP-MS). The diffusion coefficients determined at various temperatures were fitted with an Arrhenius equation. The grain boundary diffusion coefficients Dgb for W and Re at 25 GPa is determined to be 1.4 (± 0.7) x 10ˆ-7 (mˆ2/s) exp(- 485 (± 71) (kJ/mol) /RT) for W and 1.3 x 10ˆ-7 (mˆ2/s) exp(- 510 (kJ/mol) /RT) for Re, respectively. The effective diffusion distance allows modification of μ182W in considerable length scales from the core-mantle boundary through the whole Earth's history. Tungsten isotope data in modern flood basalts and oceanic island basalts reveal wide variety of μ182W ranging from negative to positive. The source regions of modern flood basalts with negative μ182W can be formed by ultra-low velocity zone just above the core-mantle boundary, whereas those of flood basalts with the positive μ182W could be originated from the large low shear velocity provinces.

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[*] Speaker

Effect of water on the rheology of clinopyroxene at high temperature and pressure

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Clinopyroxene is one of the most important constituent minerals in the lower crust and the upper mantle, and its rheological properties may determine the strength and seismic properties of the lower crust. Previous studies have shown that water content in clinopyroxene of lower crust and upper mantle varies significantly by tectonic backgrounds ranging from 50-700 ppm. However quantitative experimental investigations on the effect of water on the rheological properties of clinopyroxene have been sparse and controversy. We report here experimental deformation on synthesized clinopyroxene aggregates of varying amounts of water using a 5 GPa modified Griggs-type apparatus. Clinopyroxene aggregates of different water contents are prepared by dehydration of a water-rich natural clinopyroxene aggregates at room pressure in a mixed gaseous CO/CO2 flow buffered oven. The water contents are measured by FTIR before and after each experiment. Our results show that the strength of clinopyroxene aggregates decreases exponentially with the increase of water content. The rheological strength of clinopyroxene aggregates is reduced by about 4 times when the water content increases from 84 ppm to 662 ppm (the span of major water contents reported for clinopyroxene of lower crust and upper mantle), corresponding to a water fugacity exponent (r) value of 1.77. It is between the r values previously reported for clinopyroxene (r = 3.0, Chen et al., 2006; r = 1.4±0.2, Hier-Majunder et al., 2005). This r value is less than that reported for garnet (r = 2.4, Katayama and Karato, 2008), but larger than those reported for olivine (r = 0.7-1.25, Karato and Jung, 2003, Mei and Kohlstedt, 2000; r = 1/3, Fei et al., 2013) and plagioclase (r = 1.0±0.3, Rybacki et al., 2006). The effect of water on the rheological strength of clinopyroxene might be more significant than those for olivine and plagioclase but less significant than that for garnet. These results provide important constraints on the effect of water on the rheological properties of clinopyroxene in lithosphere.

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*Speaker

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Affect of pressure on MgO grain boundary migration; Implications for grain growth.

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Grain boundaries are an essential component of any polycrystalline assemblage. They have been shown to impact the physical characteristics of the bulk system such as electrical conductivity, reaction kinetics and impurity segregation to name just a few. Grains growth occurs in order to reduce the total grain boundary surface area of a system. We calculate the two key parameters, grain boundary energy and grain boundary mobility, which in turn define the rate at which growth occurs within a mono-phase system [Evans et al 2001].

Similar to the approaches carried out by recent Ab-Initio and molecular dynamics studies [Adjaoud et al 2012, Ghosh & Karki 2013, Verma & Karki 2010], we have calculated the energies, enthalpies and densities of states of a series of high angle grain boundary structures. The lowest energy structure for a given mis-orientation was calculated by varying the terminating atoms of each of the grain boundaries, as well as varying the relative displacement between each of the opposing grains.

Using the Nudged Elastic Band method, the conservative motion of the grain boundary is simulated by applying a theoretical shear stress to atoms that lie directly above or below one side of the grain boundary. Mobility is then ultimately defined by energy barriers that are required to move a set of atoms from one structure to another [Wu et al 2015].

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*Speaker

Synthesis of transparent nano-ceramics at high pressure and temperature

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Since the successful synthesis of transparent nano-polycrystalline diamond (NPD) by direct conversion from various forms of graphitic carbon in Kawai-type Multianvil Apparatus (KMA), we have been applying similar techniques to the synthesis of well-sintered polycrystalline bodies of some high-pressure phases. Synthesis of highly transparent nano-polycrystalline materials ("transparent nano-ceramics") has been successfully made at the ultrahigh-pressure (> 10 GPa) regime under moderate temperatures, which is attributed to a combination of rapid nucleation and slow grain growth under such conditions. Some of these ceramics have optical transparencies equivalent to those of corresponding single crystals and advanced mechanical properties in both hardness and toughness. These novel ceramics of high-pressure phases should be important for measurements of some key physical properties relevant to deep Earth mineralogy, as well as for some industrial applications such as ultra-hard materials and optical devices.

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*Speaker

Electron channeling contrast imaging of individual dislocations in geological materials using a field emission scanning electron microscope

Nobuyoshi Miyajima * [1], Yang Li [1], Sumith Abeykoon [1], Florian Heidelbach [1]

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Imaging of individual dislocations in a field emission scanning electron microscope (FESEM) is currently under spotlight. Characterization of types of the dislocation and its density is commonly performed by the diffraction contrast method, bright field and dark filed imaging in a transmission electron microscope (TEM). Also, dislocation density can be measured by indirect methods such as dislocation oxidation and etching techniques in an optical microscope and a FESEM. Here, we report electron channeling contrast imaging (ECCI) of individual dislocations in deformed ferropericlase and forsterite. The bulk specimen was polished mechanically and chemically using colloidal silica particles. The polished surface was coated with amorphous carbon. The FESEM was operated at 20 kV-acceleration voltage. The backscattered electron images were obtained at a working distance less than 10 mm. The crystal orientations of the target grains were determined by electron backscatter diffraction. Under the Bragg conditions, ECCI can provide dislocation density and the character of dislocations the in the bulk specimen. The ECCI of dislocations in a bulk specimen has many advantages over TEM in a thin foil specimen.

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*Speaker

Some recent developments in electron microscopy analysis of samples recovered from high pressure experiments

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Together with in-situ/ex-situ X-ray/neutron diffraction and optical spectroscopy observations, electron microscopy analysis of samples quenched from high pressure and high temperature plays an important role in the advancement and development of high pressure science. Over the last decade, various new methods and novel techniques for sample preparation have been introduced to our community along with the further technical development of electron microscopes. Here, we show practical examples of some new techniques/methods to examine the microtexture and chemical characteristics of recovered samples from multianvil and DAC experiments by SEM and TEM.

Cross-sectioning using ion beam provides quick and effective solutions for direct observation of recovered samples by electron microscopy. We recently introduced a JEOL cross-section polisher (CP) to prepare large-area sections for SEM-EDS, EPMA and EBSD analysis. CP uses an argon beam and gives smooth and mechanical damage- and contamination-free sections of up to 4 mm in width. We found that this technique is useful and powerful to prepare a whole cross-section across the sample chamber in a Re gasket of LHDAC samples. It is also convenient to analyze microtexture and chemical composition of recovered samples that have not been sintered well, but are porous like the case of fluid-saturated system.

Another technique we have recently introduced is osmium surface coating, which is found to be effective for SEM-EDS quantitative analysis, particularly for light elements such as oxygen, carbon and nitrogen. The Osmium coating prepared by chemical vapor deposition provides an extremely thin and uniform layer whose thickness can be controlled simply by coating time. Because of the high reproducibility and reliability of the coating process, users have no difficulty in evaluating the actual coating thickness, which enables strict and precise adsorption corrections (for the coating layer), even for low-energy characteristic X-rays. Our study shows that oxygen concentrations in silicate and oxide can be quantified correctly when using the osmium coating. The ability to accurately quantify oxygen may stimulate new applications such as the estimation of Fe2+/Fe3+ concentrations and water content in minerals.

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*Speaker

Seismic Anisotropy of the D” Layer induced by (001) Deformation of Post-Perovskite

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[2] The University of Texas at Austin – United States
[3] University of Liverpool – United Kingdom
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Crystallographic preferred orientation (CPO) of post-perovskite (Mg,Fe)SiO3 (pPv) has been believed to be one potential source of the seismic anisotropic layer at the bottom of the lower mantle (D” layer). But the natural CPO of pPv remains ambiguous in the D” layer. Here we have carried out the deformation experiments of pPv-(Mg0.75,Fe0.25)SiO3 using synchrotron radial X-ray diffraction in a membrane-driven laser-heated diamond anvil cell from 135 GPa and 2500 K to 154 GPa and 3000 K. Our results show that the intrinsic texture of pPv-(Mg0.75,Fe0.25)SiO3 should be (001) at realistic P-T conditions of the D” layer, which can produce a shear wave splitting anisotropy of _˜3.7% with VSH > VSV. Considering the combined effect of both pPv and ferropericlase, we suggest that 50% or less of deformation is sufficient to explain the origin of the shear wave anisotropy observed seismically in the D” layer beneath the circum-Pacific rim.

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*Speaker

Tuesday, morning

Experimentally determined grain growth kinetics of the spinel structure through the upper mantle to 660 km

Isra Ezad * [1], David Dobson [1], John Brodholt [1], Simon Hunt [1], Andrew Thomson [1]

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The spinel structure is common in the mantle, as aluminous MgAl2O4 stable to depths of 60 km (< 2 GPa) and silicate ringwoodite Mg2SiO4, known to exist from depths of 520 – 660 km. The spinel minerals partake in important dissociation reactions throughout the mantle:
1. CaAl2Si2O8 + 2Mg2SiO4 = MgCaSi2O6 + 2MgSiO3 + MgAl2O4;

the plagioclase to aluminous spinel transition occurs at depths greater than 20 km, (0.8 GPa).

2. MgAl2O4 + 4MgSiO3 + Mg3Al2Si2O4 + Mg2SiO4;

spinel to garnet peridotite at 2 GPa, 60 km onwards.

3a. Mg2SiO4 = MgSiO3 +MgO;

the downwelling reaction of silicate spinel ringwoodite to perovskite plus periclase, and;

3b. (Mg4,Al)(Si4,Al)O15 +MgO = Mg2SiO4 + Mg3Al2Si3O12;

the upwelling reaction for aluminous perovskite plus periclase reacting to ringwoodite plus majorite across the 660 km discontinuity.

To evaluate the importance of these dissociation reactions the diffusion driven kinetics governing them, and the grain growth of their products must be determined. We are measuring these for reactions 2 and 3.
Time series experiments have been run in the multi anvil press at University College London (UCL) at pressures less than 2 GPa for reaction 2 and at 21 and 23 GPa for reactions 3a and 3b. Both the kinetics of the reaction and the kinetics of grain growth of the inter grown reaction products are being determined.

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*Speaker

The interaction between deformation and the olivine-spinel transformation in fayalite

Tomoaki Kubo * [1], Naoko Doi [1], Masaaki Miyahara [2], Masahiro Imamura [1], Takumi Kato [1], Yuji Higo [3], Yoshinori Tange [3], Takumi Kikegawa [4]

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The non-equilibrium olivine-spinel transformation may trigger deep earthquakes and large deformation of deep slab through localized deformation enhanced by significant grain-size reduction. Therefore it is indispensable to investigate the coupling process between the transformation and deformation. In the present study, we examined creep behaviors during the olivine-spinel transformation in fayalite up to _˜14 GPa by in-situ X-ray observations.

Deformation experiments were conducted using a D-DIA apparatus in the beamline of BL04B1 at SPring-8 and NE-7 at Photon Factory. After annealing polycrystalline fayalite at _˜4 GPa and 900◦C for 2 h, we observed the olivine-spinel transformation at _˜6-14 GPa (overpressures dP of _˜1-10 GPa) and 823-1173 K with and without deformation (in uniaxial compression with constant strain rate of 3-8 x 10-5 s-1). Stress-strain and transformation-time curves were simultaneously obtained from 2D-XRD patterns and X-ray radiography images using monochromatic X-ray.

The flow stress in olivine normally increased with decreasing temperature from _˜0.5 GPa at 1173 K to _˜3-4 GPa at 823 K. Stresses in olivine, spinel, and the bulk sample were similar at the initial stage, and then spinel becomes dominant deformation phase at around 70% transformation. Spinel is stiffer than olivine in our experimental conditions. There were almost no signs for weakening and/or stress drop in the flow data. We observed grain boundary nucleation and anisotropic growth of spinel perpendicular to the principal stress direction. Nucleation was enhanced by deformation, but fine-grained reaction rims were not formed even at large dP. Thus, we did not observe clear evidences for the reaction-induced weakening as proposed in previous studies. Large dP of _˜5-6 GPa are needed to initiate transformation at 823-873 K even with deformation, in which we observed faulting across the sample associated with micro fractures. Intracrystalline lamellae in olivine developed almost parallel to the main fault. TEM analysis revealed that the thin lamellae were not composed of spinel grains, but olivine crystal with different orientation. The observed faulting and micro fractures may be caused by the deformation lamellae in olivine, however further studies with AE measurements are needed to understand the detailed process.

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*Speaker

Study Of Perovskite / Post-Perovskite Phase Transformation Mechanism By Using Multigrain Crystallography

Christopher Langrand * [1], Nadège Hilairet [1], Angelika Rosa [2], Volodymyr Svitlyk [2], David Dobson [3], Sébastien Merkel *

1,4

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At P/T conditions of the D" layer, bridgmanite transforms into its high-pressure phase of (Mg,Fe)SiO3 post-perovskite (pPv). Observations of seismic anisotropy in D" are inferred to arise from textures and microstructures within pPv. Specifically, mantle flow is though to cause pPv to deform, creating lattice-preferred orientations. However, debates emerged in the literature whether experimentally observed textures were induced by plastic deformation of the sample or by phase transformation from a previous phase and whether this could explain the observed patterns of anisotropy in the lowermost mantle.

Here, we will focus on the mechanism of transformation on a low-pressure fluoride analogue system (NaCoF3) for which it was suggested that pPv could inherit texture from the parent perovskite (Pv) phase. This inheritance of texture, combined with lattice-preferred orientation in pPv, could explain the observed patterns of anisotropy in the lowermost mantle.

We rely on a novel experimental method, Multigrain Crystallography, to characterize thousands of crystals in a polycrystalline material in-situ, as transformation proceeds. Here, we monitor individual grains during the Pv/pPv transition in NaCoF3 with P/T conditions up to 25 GPa and between 600-1500 K. We follow the distributions of grain sizes and orientations while the sample transforms from the Pv to the pPv structure, and when it transforms back from pPv to Pv. These results allow us to decipher the transition mechanism between both phases, whether it is martensitic or not, and the effect of the transformation on microstructures and grain size distributions, with important implications for our understanding of D" dynamics and anisotropy.

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*Speaker

The Mantle Transition Zone history of Tibetan chromitites: experimental constraints

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[2] Macquarie University – Australia

The Tibetan ophiolites crop out along the Yarlung-Zangbo suture zone between the Indian plate and the Lhasa block. Podiform chromitites in the Luobusha ophiolite (southeastern Tibet) are typically lens-shaped and surrounded by dunite envelopes, enclosed in well-preserved depleted harzburgites. Previous studies have shown that these chromitites were formed in shallow mantle wedge (_˜< 30 km). However, ultra-high pressure (UHP) minerals (e.g., diamond, coesite and TiO2-II), and unusual super-reducing phases (e.g., native Fe, SiC and Fe-Ni alloy), have been identified from the podiform chromitites and the host harzburgite layers. Recent studies have also revealed numerous exsolution lamellae of MgSiO3 and diopside,and rare coesite, within chromite grains. These identifications challenge the traditional hypotheses about the origin of podiform chromitites associated with ophiolites. The coesite and diopside-exsolution bearing chromitites undoubtedly experienced UHP metamorphism. However, the depth of metamorphism and origin of this exotic rock are still debatable.

In this study, we have carried out new experimental studies in the chromite+SiO2, chromite+diopside and pyrolite+chromite systems to constrain the depth of metamorphism of the Tibetan chromitites. In the chromite+SiO2 system, the experimental results demonstrate that chromite is stable up to 14 GPa and decomposes to eskolaite (Cr2O3) and a modified ludwigite-structured phase [(Fe, Mg)2(Al, Cr)2O5] at higher pressures, thus placing an approximate maximum depth for chromite crystallization and/or metamorphism. The ludwigite-structured phase has significant implications for understanding phase transformations and Cr incorporation/partitioning of minerals in the MTZ. In the chromite+diopside system, the CaFe2O4-structured phase was observed at _˜14-18 GPa, where it can contain _˜7-8 wt% of CaO and _˜3-5 wt% of SiO2. Therefore, the former presence of the CaFe2O4-structured phase from the MTZ can explain the exsolution of diopside and coesite from the chromite.

Further experiments in the pyrolite+chromite system indicate that chromite cannot coexist with the mantle mineral assemblages at depths around the 410-km seismic discontinuity. Partial-melting experiments show that garnet, rather than melt, incorporates most of the Cr available in peridotites at such depths. The results therefore indicate that chromite (or its high-pressure polymorphs) cannot directly crystallize in the deep mantle, and contradict the "deep crystallization" model for the chromitites. We suggest that the Tibetan chromitites formed under shallow conditions, and later have experienced conditions near the top of the MTZ after being deeply subducted. During the tectonics/buoyancy-driven ascent of the enclosing peridotites, the CaFe2O4-phase transformed to chromite at depths of _˜400 km, accompanied by the simultaneous exsolution of diopside and coesite, which were then preserved during transport to shallow

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[*] Speaker

depths. These observations provide a new window into the processes of mantle geodynamics, and constraints on mantle convection.

Tuesday, afternoon

Core Formation and Core Composition

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I will review some of the recent work, mostly using the laser-heated diamond anvil cell and ab initio calculations, to investigate the formation and composition of Earth's core, its secular evolution, its energetics. What we know, what we don't know, and what's in between.

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*Speaker

Light element diffusion in liquid Fe for P-T conditions of the Earth's interior

Gerd Steinle-Neumann *† [1], Esther Posner [1], David Rubie [1], Daniel Frost [1], Vojtech Vlcek [2]

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Chemical diffusion of light elements in liquid Fe plays an important role both during core formation and the growth of the inner core. However, relevant conditions are difficult to achieve in the laboratory, and first-principle determination of the diffusion constants have lacked benchmarking with experiments. Here we present results that combine experimental and computational estimates on diffusivities of Si and O in liquid Fe, covering the whole P-T range from ambient pressure to conditions of the Earth's inner core. We show that both approaches are compatible and use structural information from the molecular dynamics simulations to analyze the experimental results. Si diffuses at a comparable rate to Fe over the whole P-T range considered, which is consistent with the short-range structure in the liquid. For O in Fe, an analysis of the radial distribution function and coordination number reveals that Fe and O compress in a very different manner up to a density of approximately 8 g/cc, with initial compression primarily accommodated by an increase in coordination. This behavior can account for the very anomalous diffusion behavior observed in experiments with no appreciable P-dependence up to 25 GPa.

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[*] Speaker

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Electrical conductivity of silicate liquids at extreme conditions and planetary dynamos

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Are silicate dynamos possible? So far, planetary dynamos seated in silicate material are unknown. Several lines of evidence motivate the consideration of a silicate dynamo in the early Earth and in super-Earth exo-planets: 1) paleomagnetic evidence of a very early dynamo-generated field 2) models of the eartly thermal state of Earth in which the mantle is too hot to permit a core-generated field, and 3) the possibility of a deep, thick and long-lived basal magma ocean. The key requirement is that the electrical conductivity, s of silicate liquids be sufficiently large at the relevant high pressure-temperature conditions ($s > 1000$ S/m). Despite its importance, s of silicate liquids is unknown above a few GPa in pressure, where measured values are far too small to support dynamo activity. However, observations of reflectivity from oxide liquids in shock wave experiments suggest a different mechanism of conductivity at high pressure (electrons rather than ions). We have used ab initio molecular dynamics simulations to compute from first principles the value of s at extreme conditions in systems with compositions that are simple (SiO2) and rich (MgO-FeO-CaO-Al2O3-Na2O-SiO2). We use DFT+U with and without spin polarization combined with the Kubo-Greenwood formula. We find that the value of s exceeds the minimum requirements and that a silicate dynamo seated in a basal magma ocean is viable. We also find that the electrical conductivity shows a remarkable non-monotonic dependence on pressure that reveals connections to the underlying atomic structure, and highlights broken charge ordering as a novel compression mechanism.

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*Speaker

Nuclear resonant x-ray scattering studies under high pressure: The case for 57Fe, 119Sn, 151Eu, and 161Dy metal and their compounds

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Nuclear resonant scattering (NRS) and inelastic x-ray scattering (IXS) studies under pressure is conducted at three different beamlines at the Advanced Photon Source. Phase transitions associated with structure, magnetism, spin and valence can be studied in detail using Synchrotron M´ossbauer Spectroscopy (SMS). Key thermoelastic properties such as sound velocity, phonon density of states, vibrational entropy and specific heat, and force constant can be measured using nuclear resonant inelastic x-ray scattering (NRIXS).

We will present new results on iron, tin, europium and dysprosium based nuclear resonant studies, including isotope fractionation measurements in iron and tin compounds, and kinetics of phase transformations under varying temperature and pressure in iron. We will highlight the use of APS Hybrid fill mode for high precision Synchrotron M´ossbauer Spectroscopy.

This work is supported by U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences under contract DE-AC02-06CH11357, and the Consortium for Materials Properties Research in Earth Sciences (COMPRES) [National Science Foundation (NSF) EAR 06-49658].

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*Speaker

High-pressure equation of state of Fe-rich liquids and the solidification of molten planetary cores

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The presence of light elements such as S, Si, C, O, P, etc., can significantly modify the density, compressibility, and phase relations of the molten metallic cores in the terrestrial planets and some differentiated icy/rocky satellites. Thus, knowledge on the high-pressure properties of Fe-alloying liquids is critical to the understanding of the composition, structure, and evolution of planetary cores. In this study, we determined the sound velocity of Fe-X (X = S, Si, C, or P) liquids up to 7 GPa and 2073 K by combining the ultrasonic measurements in a multianvil device with synchrotron X-ray imaging and diffraction techniques. Combined with our density data and data in the literature, our velocity data provide tight constraints on the equations of state for Fe-rich liquids. The temperature dependence of sound velocities also provides constraints on the Anderson-Gr´uneisen parameter, from which the adiabatic temperature gradient in molten planetary cores can be calculated. We also developed a new technique to determine the high-pressure melting phase diagram of Fe-light element alloys utilizing the ultrasonic sound wave propagation through the sample. With this technique, we have determined the phase diagram of the Fe-P system up to 7 GPa. Comparing adiabatic temperature gradients derived from our velocity data with the pressure dependences of liquidi for metallic cores, our results point to complex solidification histories of metallic cores, depending on the pressure and the type and abundance of light elements present in planetary cores.

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[*] Speaker

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Phase transition boundary between fcc and hcp structures in the system Fe-Si and its implications for thermodynamics of silicon-bearing Earth's core

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The phase transition between a face-centred cubic (fcc) and hexagonal close-packed (hcp) structure in Fe-Si alloys were examined in an internally resistive heated diamond anvil cell (DAC) under high-pressure (P) and -temperature (T) conditions with in-situ synchrotron X-ray diffraction (XRD). High pressure was generated in a DAC with a pair of diamond anvils with a culet size of 300 μm or 150-450 μm beveled depending on the pressure range. The starting material was Fe-4wt%Si, sandwiched between SiO2 glass layers which served as a pressure transmitting medium and thermal insulator. High temperature was achieved with an internal resistive system. A 5-7μm thick sample foil was placed in the sample chamber and resistively heated by directly applying a DC voltage by an external power supply. The temperature was measured by a spectral radiometric system as in conventional laser heating experiments. In-situ XRD experiments were conducted at the beamline ID27, European Synchrotron Radiation Facility. We placed tight constraints on the P-T locations and the width of the phase loop of the fcc-hcp transition. From the precisely constrained phase loop, we have constructed a thermodynamic model for the fcc-hcp transition in the Fe-Si system. The model includes P-T dependence of the mixing properties of Fe-Si alloys. We then extend the discussion to the thermodynamics of melting in the system Fe-Si. The compositions of coexisting liquid and solid (fcc or hcp) have been reported to be close ($<$ 1 wt%Si) at pressures higher than 50 GPa, and we evaluated the thermodynamic parameters which reproduce those melting relations. We will show our experimental data and thermodynamic modelling, and then further discuss resulting implications for Earth's core.

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[*] Speaker

Thermoelastic properties of hcp-Fe-Si-C-S alloys under the Earth's inner core conditions

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Geophysical and cosmochemical models constrain the inner core to be composed mainly of iron and few percent light elements including Si, S, C, and H. However, mineral physics results do not agree with the seismological observations of both density and sound wave velocities in the inner core (Vočadlo, 2007; Vočadlo *et al.*, 2009; Belonoshko *et al.*, 2007; Martorell *et al.*, 2013). Recent studies suggest a candidate for the inner core could be *hcp* iron alloyed with light elements (Li. *et al.*, 2001; Antonangeli, *et al.*, 2010; Hirose, *et al.*, 2013). Using *ab initio* molecular dynamics calculations, we have studied the structure and elastic properties of *hcp*-Fe alloys at 360 GPa up to the melting temperature. A ternary *hcp*-Fe30Si1C1 alloy was found to match both the inner-core density and sound velocities. We also found other possible ternary and quaternary candidates based on a solid solution model, where carbon is always a necessary component to be in agreement with the seismic observations. These Fe-C-X compositions provide a new understanding of the Earth's core with important geodynamic implications.

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*Speaker

Triple point hcp-fcc-liquid in pure Fe phase diagram determined by in-situ XANES diagnostic

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[8] Earth Life Science Institute (ELSI) – Japan
[9] Ehime University (Ehime Univ.) – Japan

Iron is the main constituent of planetary cores. Studying its phase diagram under high pressure is mandatory in order to constrain properties of planetary interiors, and to model key parameters such as the generation of magnetic field.

Strong controversy is still large regarding the melting curve of pure Fe. In contrast, throughout the literature, we can observe an overall agreement on the melting temperature of many iron alloys under extreme conditions, with results within mutual uncertainties, irrespectively of the melting diagnostics. However, a controversy has been recently pointed out on the case of pure iron, with XANES measurements (Aquilanti et al, PNAS, 2015) in open disagreement with previous results by x-ray diffraction (Anzellini et al, Science, 2013).

We performed in situ XANES experiments on the beamline ID24, using the available experimental setup combining dispersive absorption set up and laser heated diamond anvil cell. Samples

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*Speaker

recovered from high temperature-high pressure experiments were probed by XRD and FIB techniques, to assess the melting criterion derived by XANES change. Low melting temperatures, corresponding to the ones described in Aquilanti et al, 2015, are systematically related to the presence of Fe3C, that is to say carbon contamination from the diamonds, evidenced by XRD and XANES.

Triple point in the Fe phase diagram is located at 105 (±10) GPa and 3600 (±200) K. This seems to be related to a small kink in the melting curve around the triple point. Over the triple point, melting seems to be in relative agreement with previously published XRD melting curve (Anzellini et al, 2013). The refinement of the Fe phase diagram could be used to compute thermodynamic model for planetary cores.

Sound velocity of iron-light element compounds and composition of the inner core

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The seismological and mineral physics studies indicate that the Earth's core consists of iron-nickel alloys containing light elements. The major candidates of the light elements in the core may be S, Si, O, and H. Recent studies on melting of the Fe-Si-O and Fe-Si-S-O systems revealed that Si and O are mutually exclusive in metallic liquid [1], and silicates such as SiO2 (e.g., [2]) or FeSiO3 were precipitated during cooling of the liquid core. Therefore, the metallic inner core crystallizing from liquid outer core should be composed of ether Fe-O-S or Fe-Si-S alloys.
Our sound velocity measurements revealed that both compressional velocity (Vp) and density of pure hcp-Fe are greater than those of the PREM inner core indicating that the major light elements in the inner core must reduce both compressional velocity and density of hcp-FeNi alloy [3]. Our sound velocity measurements of iron-light element compounds revealed that S, Si and H can meet with this requirement [3], whereas the sound velocity of FeO is very high compared to the PREM inner core [4]. Thus, O may not be the major light element of the inner core.

The experiments on the solid-liquid partitioning of S and Si together with the sound velocity measurements of iron-light element alloys at high pressure and temperature revealed that the major element of the inner core is Si whereas that of the outer core is S, and an iron-nickel alloy with about 3-6 wt.% of Si and 0.1 wt. % of S with additional Ni of 0_˜8 wt.% can explain both the density and compressional velocity of the PREM inner core assuming that the inner core does not contain hydrogen.

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*Speaker

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Formation of non-stoichiometric fcc and hcp FeHx at high pressure and temperature conditions

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Hydrogen is one of the likely light elements in the Earth's core but the phase relation of FeHx alloy is not well known yet, due to experimental difficulties. Double hexagonal closed packed (dhcp) FeH was suggested to be stable, at least to 136 GPa based on static compression at room temperature, whereas the stabilities of face centered cubic (fcc) and hcp FeHx were also reported. The phase relation in FeHx, in particular for a hydrogen depleted composition ($x< 1$) and at high temperatures, remains to be examined. Here we performed experiments on FeHx ($x< 1$) using a laser-heated diamond anvil cell (LH-DAC) and observed its phase relation up to 136 GPa and 2000 K by X-ray diffraction measurements. Rhenium gasket was used without hydrogen sealing; that is, system was open for hydrogen. Dhcp FeHx (x_˜1) was synthesized under 5 GPa by annealing. However, the diffraction peaks from dhcp FeH became weak over 20 GPa, and then dhcp to fcc phase transition took place up to 33 GPa, in which $x = 0.9$ to 1.0. With further compression, the fcc phase was preserved, although x decreased to 0.7 at 93 GPa. During heating below 1800 K at 65, 70, and 122 GPa, hcp FeHx formed and the fcc phase gradually disappeared probably because of hydrogen escape from a sample chamber. The amount hydrogen in this hcp phase was lower than 0.6 and decreased with increasing laser output power. Our result indicated that both fcc and hcp phases could have stability fields in the Fe-H binary system. Because hydrogen concentration required to account for the density deficit is 0.6 (_˜1 wt.% H) in the outer core and 0.1 in the inner core, hcp FeHx is the most important compound in order to test the hypothesis that hydrogen is in the Earth's core.

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[*] Speaker

Sound velocity and elastic properties of liquid Fe–Ni–Si at high pressure

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Sound velocity, density, and elastic properties, such as bulk modulus, of liquid Fe-alloys at high pressure give us important information to constrain interior structures and composition of molten cores of terrestrial planets. Si is one of the major light elements in the planetary core. Here, we measured compressional wave velocity (Vp) and density of liquid Fe–Ni–Si and studied the effect of pressure, temperature, and Si content on these properties.
Sound velocity and density of liquid Fe52Ni10Si38 was measured up to 12 GPa and 2100 K using ultrasonic pulse-echo method and X-ray absorption method, respectively. The measurements were carried out at BL04B1 and BL22XU beamlines, SPring-8.

The measured Vp of Fe–Ni–Si is larger than that of liquid Fe (Jing et al. 2014) and Fe–Ni (Kuwabara et al. 2016) in all the pressure range studied. The effect of Si on the Vp is opposite to that of S at present pressure conditions. The Vp of liquid Fe–Ni–Si decreases slightly with increasing temperature and the dVp/dT of this study is in agreement with that measured at ambient pressure (Williams et al. 2015). The adiabatic bulk modulus (*Ks0*) at ambient pressure and its pressure derivative (*Ks'*) were obtained by fitting the *Vp* data using the Birch-Murnaghan and Vinet equation of state. The obtained *Ks0* of liquid Fe–Ni–Si is close to that of liquid Fe–Ni (Kuwabara et al. 2016). The calculated density from the *Ks0* and *Ks'* shows a good agreement with the directly measured density.

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*Speaker

Wednesday, morning

Immiscible Hydrocarbon Fluids in the Mantle

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[2] Johns Hopkins University (JHU) – Baltimore, USA, United States

The cycling of carbon between Earth's surface and interior governs the long-term habitability of the planet. But how carbon migrates in the deep Earth is not well understood. In particular, the potential role of hydrocarbon fluids in the deep carbon cycle has long been controversial. Here we show that immiscible isobutane formed *in situ* from partial transformation of aqueous sodium acetate at 300 °C and 2.4 - 3.5 GPa. These observations complement recent experimental evidence for immiscible methane-rich fluids at 600 – 700 ◦C and 1.5 – 2.5 GPa and the discovery of methane-rich fluid inclusions in diamonds and metasomatized ophicarbonates at peak metamorphic conditions. Theoretical predictions indicate that high pressure strongly opposes decomposition of isobutane and that it can coexist in equilibrium with silicate mineral assemblages. Decomposition at lower pressures could provide a source of abiogenic methane in the deep crust. Consequently, a variety of highly mobile, immiscible hydrocarbon fluids might be facilitating major carbon transfer in the deep Earth carbon cycle. doi: 10.1038/ncomms15798

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Coupling deformation under high pressures, synchrotron X-rays and acoustic emissions monitoring for the study of deep earthquakes

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The coupling of synchrotron radiation to the Deformation-Dia was a breakthrough for in studies of rheological properties under extreme conditions of pressure and temperature (up to 18-20 GPa and to 2000 K). Recent developments using acoustic emissions monitoring have significantly widened the range of problems that can be addressed with these experiments, including the study of phase transformations under high pressures and associated mechanical instabilities. Synchrotron X-ray diffraction and radiography allow measuring in-situ sample macroscopic strain, lattice preferred orientations, and lattice strains as proxy for stresses, from grain scale to sample scale. In addition, acoustic monitoring now allows studying crucial characteristics of 'brittle-like' events within the samples.

These developments bring for instance new clues on how deep earthquakes (> 50 km depth) could be triggered. At these confining pressures earthquakes cannot be explained by conventional rupture theories, and the causes for the seismicity occurring down to below 600 km depth in the earth are still unclear. We will present results from recent studies (e.g. Ferrand et al, 2017, Gasc et al, 2017, Incel et al, 2017) relevant for subduction zones intermediate-depth seismicity, that highlight how the interplay between mineralogy, elastic and plastic properties of minerals can produce micro-quakes in a laboratory. These methods open the door to a wide range of further studies in high pressure mineral physics.

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S. Incel, N. Hilairet, L. Labrousse, T. John, D. Deldicque, T. Ferrand, Y. Wang, J. Renner,

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*Speaker

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Water and carbon cycle in global-scale mantle dynamics modeling

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Here we show recent accomplishments on mantle water cycle with vigorous surface plate motion in numerical mantle convection simulations with experimentally-determined water solubility maps, which are an efficient occurence of surface plate motion in hydrous mantle convection and its influence to water absorption in the deep mantle and ocean-plate-mantle-core system evolution. On first accomplishement, the efficient plate motion caused by water-dependnet rheology may enhance the heat transfer in mantle convection so that the mantle transitin zone can absorb the huge amount of water. As a result, the mantle water content may be rapidly increased as a function of time when the surface plate motion is efficiently ocurred, which suggests that the water-dependent rheology may work for a positive feedback of mantle water cycle but a negative feedback to thermal state in the mantle. Second, the evolution of mass of ocean water is included in the hydrous mantle convection model with parameterized core heat balance. Using this improved model, the total amount of water in the entire Earth's system may be 4_˜5 Ocean Masses suggested from early plananetary formation rather than 2 Ocean Maasses in tradiational solid Earth geodynamics. This also causes the water solubility maps of hydrous mantle minerals that may have the large value in the mantle transition zone. This suggests that the large amount of water should be found in the present Earth but it is not very clear when and where the water can be distributed in the early Earth formation. In addition, if possible, we also indicate an effects of phase-H in the hydrous mantle convection model as well as show the preliminary result of the carbon cycle model across the surface and its influence to surface environement, which strongly affects the volcanic degassing from deep interior to surface.

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*Speaker

High-pressure phase transitions in AlOOH and FeOOH

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Hydrogen is transported into deep Earth's mantle regions as a form of hydrous minerals via subduction of oceanic plates. CaCl2-type hydroxides such as (Mg,Si)OOH phase H, δ-AlOOH, and their solid solutions were reported to have large P–T stability fields that encompass conditions representative of the lower mantle, implying the possibility that surface water may be transported as far as the core–mantle boundary. Also, compositional analysis of phase H grains synthesized from natural serpentine shows a presence of the FeOOH component in this phase (Nishi et al., 2015). This result suggests that phase H and δ-AlOOH would also form solid solutions with ϵ-FeOOH, since ϵ-FeOOH is isostructural to phase H and δ-AlOOH. In addition, ab initio calculations have predicted that some CaCl2-type hydroxides transform to the pyrite-type structure at higher pressures (Tsuchiya and Tsuchiya, 2011). Here we report the stability of AlOOH, FeOOH, and their solid solutions based on in-situ X-ray diffraction (XRD) measurements combined with multi-anvil apparatus and laser-heated diamond anvil cell techniques. The XRD patterns showed clear diffraction peaks that can be accounted for by the pyrite-type structure, which matches that predicted by theoretical calculations (Nishi et al., 2017). We also found that δ-AlOOH transforms to the pyrite-type structure at higher pressures. Further experiments revealed that solid solutions over a wide composition range in the system AlOOH–FeOOH were maintained through the spin transition of Fe and the structural phase transition from CaCl2-type to pyrite-type structure. Based on these experimental and theoretical results, we will disscuss stability of the hydrous phase in the lower mantle and the deep interiors of other planets.

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*Speaker

Exploring new phenomena in salty ices and ice clathrates under planetary conditions

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Compressed water is overspread on Earth at depth and in the extra-terrestrial space, both interstellar and on outer planets and moons. Under the extreme p-T conditions experienced in these celestial bodies water displays an incredibly rich phase diagram, anomalous dynamical properties, proton conductivity, and unusual affinity for both ionic and gaseous species. In this talk I will review our recent experimental results on, pure1,2, salt-doped (LiCl, NaCl, KCl)3,4,5, and gas (H2, CH4)6- "stuffed" ices under the extreme conditions experienced in the ice bodies of our solar system.

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[6] U.L. Ranieri, et al., Nat. Comm., submitted (2017).

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*Speaker

Experimental study on the stability of methane hydrate under high pressure and high temperature

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Methane hydrate (MH) is thought to be an important constituent of icy planets and their satellites, such as Neptune, Uranus and Titan. It is a clathrate compound composed of hydrogen-bonded water cages and methane molecules included in the cages. MH has an sI cage structure composed of two 12-hedral and six 14-hedral components in a unit cell at low ($<$ 0.8 GPa) pressures and room temperature. It transforms to an sH cage structure composed of three 12-hedra, two modified 12-hedra, and a 20-hedra at approximately 0.8 GPa, which further transforms to a filled-ice Ih structure at approximately 1.8 GPa (Loveday et al., 2001). The Ih structure consists of an ice framework similar to ice Ih and voids that are filled with methane molecules. Although the sequence of the phase transitions with pressure have been studied well at room temperature, there are only a few studies that addressed the stability of MH under high pressure and high temperature. A recent work by Bezacier et al. (2014) studied the decomposition temperatures of MH at pressures between 1.5 and 5 GPa. They demonstrated that it decomposes into solid methane and liquid water at temperatures close to the melting curves of ices, which is, however, not consistent with an earlier report by Kurnosov et al. (2006). In addition, the pressure range of these previous studies is only limited to $<$ 5 GPa. Therefore, a further investigation is needed to understand the stability and physicochemical behavior of MH under extreme conditions corresponding to the mantle of giant icy planets. In this study, we carefully investigated the stability of MH under 2-51 GPa and 298-653 K using in-situ Raman spectroscopy and X-ray diffraction. Prior to in-situ high P-T experiments, the typical C-H vibration modes and their pressure dependence of MH were measured at room temperature using Raman spectroscopy to distinguish MH from solid methane which would appear through the decomposition of MH into solid methane and ice VII. The results of high P-T experiments showed that MH decomposes into solid methane and ice VII at temperatures considerably lower than the melting curves of solid methane and ice VII in the pressure range of 2-51 GPa. This suggests that MH is unlikely to be stable in the mantle of giant icy planets such as Neptune and Uranus.

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[*] Speaker

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The effect of hydration on the elastic properties of ringwoodite at transition zone pressures

Kirsten Schulze * [1], Hauke Marquardt [1], Alexander Kurnosov [1], Takaaki Kawazoe [1], Tiziana Boffa Ballaran [1]

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Mineral physics experiments have shown that ringwoodite can incorporate significant amounts of hydrogen into its crystal structure. Since ringwoodite is considered to be the most abundant mineral in the Earth's transition zone below 520 km depth, this opens the possibility for the presence of large amounts of water-equivalents in the mantle. This hypothesis is supported by the detection of _˜1.4 wt% H20 in a mantle ringwoodite found as a diamond inclusion (Pearson et al. 2014). The actual amount of 'water' in the transition zone, as well as its spatial distribution are still controversially discussed. A promising way to detect and map hydration of the transition zone is based on seismological observations, as mineral physics findings predict a significant reduction of seismic wave velocities of ringwoodite upon hydration. However, differences in predicted pressure effects complicate a reliable quantification of this effect at mantle transition zone pressures and temperatures, precluding any conclusive estimate of the hydration state of the transition zone.

Here we report results of an extensive HP/HT single-crystal Brillouin spectroscopy and X-ray diffraction study performed on four samples of ringwoodite with a Fo90 or Fo100 composition and a hydration state of 0.44 - 3.40 mol/L, equivalent to 0.21 - 1.71 wt% H2O.

To ensure identical experimental conditions and minimize relative uncertainties, all four samples were loaded in the same pressure chamber of a diamond anvil cell. Brillouin spectroscopy and X-ray diffraction were performed up to a pressure of 22 GPa. Further experiments were carried out up to 630 K temperature at pressures of the transition zone.Our comparative study indicates that the effect of hydrogen on the elastic properties is significantly smaller than predicted by previous studies. In particular, a reduction of the effect of hydration with increasing pressure is observed. At pressures equivalent to the lower transition zone, the velocity reduction caused by 2 mol/L of water is less than 1%.

For a pyrolitic mantle composition, ringwoodite is expected to constitute _˜56% by volume. Therefore, given the small effect of hydration on the elastic properties of ringwoodite, even large amounts of water in the transition zone mantle might be seismically indistinguishable from an anhydrous mantle.

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[*] Speaker

Wednesday, afternoon

Eutectic melting in the MgO-SiO2 system and its implication to Earth's lower mantle evolution

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Eutectic melting curves in the system MgO-SiO2 have been experimentally determined at lower mantle pressures using laser-heated diamond anvil cell technique. We investigated eutectic melting of bridgmanite + periclase in the MgO-MgSiO3 binary and bridgmanite + stishovite in the MgSiO3-SiO2 sub-system as the simplest models of natural peridotite and basalt. Eutectic melting was detected on the basis of the thermal perturbations (i.e. melting plateau) during the experiments, but also by textural and chemical analyses of recovered samples. We also performed a suite of sub-solidus experiments to compare and bracket the results.
The melting curve of model basalt occurs at lower temperatures, has a shallower dT/dP slope and slightly less curvature than the model peridotitic melting curve. Overall, melting temperatures detected in this study are in good agreement with previous experiments and *ab initio* simulations at ˜25 GPa (Liebske and Frost, 2012; de Koker et al., 2013). However, at higher pressures our melting curves are systematically lower than curves extrapolated on the basis of thermodynamic modelling and atomistic simulations. Compared to previously published solidus curves obtained for natural basalt and peridotite (e.g. Fiquet et al., 2010; Andrault et al. 2011; Andrault et al. 2014 and Pradhan et al. 2015) the melting curves from this study are consequently higher.

Based on the comparison of the curvature of the model peridotite eutectic relative to an MgSiO3 melt adiabat, we infer that crystallization in a global magma ocean would begin at ˜100 GPa rather than at the bottom of the mantle, allowing for an early basal melt layer. The model peridotite melting curve lies ˜500 K above the mantle geotherm at the core-mantle boundary, indicating that it will not be molten. The model basalt melting curve intersects the geotherm at the base of the mantle, and partial melting of subducted oceanic crust is therefore expected.

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[*] Speaker

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In order to improve the thermal distribution during long subsolidus experiments and greatly reduce the temperature gradients, we have also developed a microfabrication technique for total metal-encapsulation of silicate samples together with a numerical 2D thermal distribution model which simulates experimental conditions with various pressure cell geometries.

Densification mechanisms of amorphous silicates at high pressure and temperature

Alisha Clark *† [1,2], Guillaume Morard [3], Yann Le Godec [3], Nicolas Guignot [4], Andrew King [4]

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The interconnected network of SiO4 tetrahedra is the main structural feature of silicate glasses and liquids at pressures up to 15 GPa. Polymerized silicate glasses (SiO2-MgSiO3 binary) exhibit unusual volumetric and elastic properties at high pressure and room temperature, including the observation that compressibility increases or is weakly pressure dependent on compression. The anomalous behavior of polymerized silicate glasses is consistent with densification being controlled by network flexibility, rather than the compression of interatomic distances as exhibited in their crystalline counterparts. Moreover, depolymerized compositions (MgSiO3 – Mg2SiO4 binary) have anomalously high proportions of interconnected SiO4 tetrahedra compared to the predictions based on stoichiometry, suggesting that network flexibility may play an important role in the high pressure properties of depolymerized amorphous silicates as well. To determine the P-T-X range over which network flexibility controls densification, we measure combined *in situ* X-ray diffraction and microtomography datasets at elevated pressure and temperature in the Rotational Tomography Paris-Edinburgh Cell at the SOLEIL synchrotron for a suite of silicate glasses spanning the SiO2-MgSiO4 binary. Simultaneous acquisition of X-ray diffraction on a large Q-range (up to 160 nm-1) and 3D tomography were performed under extreme conditions, permitting direct comparison of density from volumetric measurements with changes in atomic structure. We use these results to investigate the role of network flexibility and polyamorphism in the anomalous high pressure behavior.

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Density and structure of amorphous silicates at high pressure conditions

Sylvain Petitgirard * [1], Wim Malfait [2], Ilya Kupenko [3], Christoph Sahle [4], Ines Collings [4], Christopher Weis [5], Georg Spikermann [6], Ryosuke Sinmyo [7], Eleanor Jennings [8], Ingrid Blanchard [8], Christian Sternemann [5], Max Wilke [6], David Rubie [8]

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[8] Bayerisches Geoinstitut (BGI) – Germany

Modelling the formation and evolution of the deepest parts of the Earth through time requires the densities of solids and melts to be constrained. Other properties such as the structure and viscosity of high pressure melts are also needed to undersatnd the fate of deep mantle melts. The main parameter controlling the entrainment or settlement of matter in the lowermost mantle and the possible deep magma ocean formation is the density contrast between solid and magma. To measure the density of amorphous silicates, we have adapted the X-ray absorption method to the diamond anvil cell confinment to enable density measurements of silicate glasses to be made to unprecedented conditions of high pressure [1]. We have consequently measured the densities of SiO2 and MgSiO3 glasses up to 110 and 127 GPa, respectively. We found that the glass and melts at CMB pressure can be as dense as their counterpart solids. Recently we extended the data to iron-bearing compsoition (Mg0.7Fe0.3SiO3) to 150 GPa and we aim at forming a density model for amorphous silicate in the MgO-FeO-SiO2 system.

To understand the changes in the structure associated with such high densifictaion we measured the changes of the Si L2,3-edge and O Kedge in SiO2 glass under pressure by means of X-ray Raman scattering specrtoscopy up to 110 GPa. Together with the density measurments, we are able to give a framework for the densification of SiO2, with the appearance of a "5-fold-like" strutcure bewteen 20 and 60 GPa that accomodate the transition from 4-fold to 6-fold coordination.

These new data bring a deeper knowledge of the density, structural, polymerization and viscosity changes of silciate magmas at lower mantle pressures.

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*Speaker

Structure of silicate glasses up to 172 GPa

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The physical properties of silicate melts at temperature and pressure conditions of the Earth's mantle have a fundamental influence on the chemical and thermal evolution of the Earth. However, direct investigations of melt structures at these conditions are experimentally very difficult or even impossible with current capabilities. In order to still be able to obtain an estimate of the structural behavior of melts at high pressures and temperatures, amorphous materials have been widely used as analogue materials.

Here we report experimental investigations of the structural behavior of glasses of SiO2 up to 172 GPa, MgSiO3 up to 135 GPa, and Mg2SiO4 up to 140 GPa using X- ray total scattering and pair distribution function analysis. To further understand ultra high pressure behavior we have investigated GeO2 glass, as an analogue for SiO2 glass, up to 85 GPa. The very high pressure range for these measurements were enabled by the newly commissioned multichannel collimator setup at GSECARS, APS, which significantly reduces the amount of diamond Compton scattering. This facilitates the collection of total x-ray diffraction patterns up to a maximum Q of 15 A-1 at very high pressures.

The data clearly shows changes from 4- to 6-fold coordination of Si, which is completed around 40-60 GPa, depending on composition, in agreement with previous reports. GeO2 shows an increase to 6-fold coordination already about 25-30 GPa. At higher pressures, after the change to 6-fold coordination, the glasses show smooth changes in structure factors S(Q) and pair distribution functions g(r). The Si coordination number gradually increases to about 7.2 at 172 GPa for SiO2 with no apparent discontinuity.

We will present experimental data, discuss densification mechanisms and differences of the various glass compositions at high pressures. The goal is to establish a framework for silicate glass structures as analogue materials for silicate melts to understand the deep Earth's interior.

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*Speaker

The High-Pressure Structure of Silicate Melts and the Impact on Magma Ocean Evolution

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The early evolution of terrestrial planets is strongly influenced by the high P-T properties of silicates liquids. Planets like Earth are expected to experience multiple giant impacts during accretion which bury tremendous heat sufficient to melt a significant fraction of the rocky mantle and produce deep magma oceans. From this initial molten state, the mantle cools and solidifies, but its evolutionary path is highly uncertain. This coupled thermodynamic and fluid dynamic process is highly sensitive to the thermophysical properties of both liquid and solid along the melting curve. The curvature and slope of the melting curve, as compared to the adiabatic profiles of the magma ocean, directly determine the depth of initial crystallization. Two competing endmember hypotheses argue that the mantle would crystallize from the bottom-up (e.g. Andrault et al., 2011) or the center-outwards (e.g. Stixrude et al. 2009), and resolving this puzzle requires a careful assessment of the properties of high pressure melts. We thus develop a new high-pressure equation of state (EOS) for liquids and combine it with a simple model for the structural degrees of freedom of silicate melts. Our new liquid-specific EOS, RTPress, gives a high-pressure extension of Rosenfeld Tarazona model. We apply this model to molecular dynamics (MD) simulations of MgSiO3 melt (Spera et al. 2011), and validate it against the experimental shock wave Hugoniot of enstatite glass (Mosenfelder et al. 2009). The magma ocean crystallization depth is obtained by comparing the adiabats given by our model with the mantle melting curve. There is not a current consensus about the shape of the deep mantle melting curve, with dramatic differences in the degree of curvature across experiments and simulations. To help resolve this issue, we adopt an independent thermodynamic approach of modifying the pure MgSiO3 melting curve to account for realistic mantle chemistry. The structure of these melts play a central role in determining their entropy, which directly influences the slope of the melting curve. By analyzing previous MD studies, we model the configurational entropy effect on the shape of the mantle liquidus. The non-negligible curvature of the resulting liquidus is shown to favor center-outwards, rather than bottom-up, crystallization.

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*Speaker

High Speed X-ray imaging for studying behavior of liquids at high pressures and high temperatures

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In situ characterization of materials under conditions of high pressure and high temperature (HP-HT) are of great interest in planetary and materials sciences as well as physics and chemistry. Upon the last decade, many efforts have focused on the development of *in situ* three-dimensional (3D) tomographic imaging at HP-HT, which enable nondestructive investigations of heterogeneous structures of materials [e.g. Wang et al. 2005, Philippe et al. 2016]. X-ray imaging is one of the most powerful tools for investigating the behavior and properties of liquids (i.e. viscosity, surface tension on a liquid-liquid interface or immiscibility of liquids). A critical parameter for the accurate characterization of these properties in liquids is the time resolution (e.g. acquisition time) at which changes can be observed, detected and/or measured [e.g. Kono et al 2015]. We have implemented high speed X-ray tomography at HP-HT on the Psiché Beamline at Soleil Synchrotron (France). Using pink beam through a Paris-Edinburgh Press, we were able to increase the speed by 100 compared to the current state of art (i.e. from 15 min to < 10 s). In complementary, high speed 3D tomography can be integrated with combined angle- and energy-dispersive structural analysis and refinement acquisitions [CAESAR, Wang et al. 2004], offering the possibility to study material/liquids structures at the micro and atomic scales. Here, we will present first measurements of silicate melt propagation through a solid silicate matrix at HP-HT and discuss its applications in Earth sciences as well as further developments for higher speed acquisition (< 1s) in the near future on Psiché Beamline.

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Experimental evidence supporting global melt layer at the base of the Earth's upper mantle

Geeth Manthilake * [1], Damien Freitas [1], Federica Schiavi [1], Julien Chantel [2], Nathalie Bolfan Casanova [1], Mohammed Bouhifd [1], Denis Andrault [1]

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The globally observed reduced seismic wave velocity (-4% for Vs) at mantle depths of 350-410 km, has been attributed to the presence of melt 1–3. **It has been proposed that mantle upwelling and subsequent release of free fluids, when hydrous wadsleyite transforms into olivine, is responsible for melting at the base of the Earth's upper mantle** 4. **Partial melting of peridotite at corresponding pressure and temperature, however, requires a substantial contribution from volatile components** 4 **and the produced melt needs to be neutrally buoyant in order to remain at the base of the upper mantle** 5. **In this study, we experimentally reproduced the phase transformation in the upwelling mantle at relevant mantle conditions and investigated the sound wave velocity during partial melting of hydrous peridotite. Our seismic velocity model indicates that the observed -4 % Vs anomaly can be explained with 0.7 melt fraction in peridotite. The resulting melt contains up to and 33 wt. % FeO. Based on the effect of H2O on melt density, the water contents of gravitationally stable melt are estimated to be within 13.3-19.3 wt. % for 0.7 % melt fraction. This translates the corresponding water content in the mantle transition zone (MTZ) to 0.22 ± 0.04 wt. %, significantly lower than the near water saturated conditions depicted by previous studies** 6,7.

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Computational and experimental studies of iron-bearing carbonates and silicate glasses at lower mantle pressures

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Decomposition of carbonates may be responsible for creating silicate melts within Earth's mantle by lowering the melting temperature of surrounding rock. Characterizing the stability of carbonate phases is therefore a necessary step towards understanding the transport and storage of carbon in Earth's interior. Dolomite is one of the major mineral forms in which carbon is subducted into Earth's mantle. Although iron-free dolomite is expected to break down upon compression, high-pressure polymorphs of iron-bearing dolomite may resist decomposition. Using a genetic algorithm that predicts crystal structures, we found a monoclinic phase with space group C2/c that has a lower energy than all previously reported dolomite structures at pressures above 15 GPa, where the substitution of iron for magnesium stabilizes monoclinic dolomite with respect to decomposition at certain pressures of the lower mantle. Thus, an iron-bearing dolomite polymorph may be an important carbon carrier in regions of Earth's lower mantle.

The depth at which carbonates will decompose is dependent on the age, temperature and density of subducting slabs. Decarbonation reactions may lower the melting temperature of surrounding rocks to produce silicate melts. In regions of the mantle where silicate melts may exist, it is important to understand the physical properties and dynamic behavior of the melts because they affect the chemical and thermal evolution of its interior. Composition, degree of polymerization, and iron's spin state affect such properties. The behavior of iron in silicate melts is poorly understood but, in some cases, may be approximated by iron-bearing glasses. We measured the hyperfine parameters of iron-bearing rhyolitic and basaltic glasses up to _˜120 GPa and _˜90 GPa, respectively, in a neon pressure medium using synchrotron M´ossbauer spectroscopy. The spectra for rhyolitic and basaltic glasses are well explained by three high-spin Fe2+-like sites with distinct quadrupole splittings, reflecting the influence of evolving coordination environments with pressure. With the assumption that coordination environments in silicate glasses may serve as a good indicator for those in a melt, this study suggests that ferrous iron in chemically–complex silicate melts likely exists in a high-spin state throughout most of Earth's mantle.

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Thursday, morning

Picosecond Acoustics : a way to Thermodynamical Properties of Solids and Liquids at Extreme Conditions

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Based on the original combination of picosecond acoustics and diamond anvils cell, hypersonic sound velocities of liquids and solids under extreme conditions can be accurately measured [1]. Picosecond acoustics is a time-resolved optical pump-probe technique, contactless and non-destructive, analogous in many aspects to the classical ultrasonic pulse-echo technique. It permits the study of ultrafast phenomena in micrometric samples or thin films. In addition to time of flight measurements in the ps range, it can provide phonon surface imaging as a function of time, or time-resolved stimulated Brillouin scattering.
This laser acoustic technique can be applied to many materials and enables the determination over and extended pressure and temperature range of the melting curve and phase diagram, the equation of state for liquids, the complete set of elastic constants for single crystals.

To illustrate the capability of this technique, results will be presented for different types of studies and materials: complete elastic tensor on single-crystalline sample (Si) up to 10 GPa [2], longitudinal sound velocity on polycrystalline samples (Fe) at Mbar pressure [3], sound velocity and melting curve of metallic liquids (Hg[4], Ga [5], Rb, Cs) at high pressure and temperature, and Poisson ratio as a function of pressure for hydrogen [6].

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Development of ultrasonic measurement technique under lower mantle conditions

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Elasticity data on mantle minerals under high pressure and high temperature are critical to interpret the seismic velocity and density profiles in the Earth's deep interior. However, ultrasonic measurements of elastic wave velocities under high pressure and high temperature have been limited to those corresponding to the mantle transition region ($<$ 20GPa, $<$ 1673K), because of the technical difficulties. Since only a small sample can be used in the experiment under the lower mantle conditions, ultrasonic echoes are very weak and cannot perform a precise elastic measurement. In this study, to overcome this problem, the high-frequency arbitrary waveform generator, post amplifier and high-speed semiconductor relay were installed in BL04B1 at SPring-8. A tiny pure polycrystalline alumina (a-Al2O3) rod (Diameter = 1.0mm, Length = _˜0.5mm) was used as the test sample, because alumina is a very hard and stable material under high pressure and temperature conditions. An assembly of eight cubic anvils of WC with edge length of 26 mm and truncated corner of 3.0 mm has been used in Kawai-type multi-anvil apparatus (SPEED-1500). Travel times for both P- and S-waves passing through the sample were measured by the ultrasonic interferometry, and each sample length under pressure was determined from the X-ray image of the sample using a high-resolution CCD camera. At the same time, X-ray diffraction data from the sample were acquired, and the generated pressures were monitored throughout the run. We have successfully measured elastic wave velocities of alumina up to _˜30GPa, which corresponds to the lower mantle P-T condition. The waveforms observed very clear, and the echoes of P-wave and S-wave were identifiable at high pressure and high temperature. Precise elastic wave velocity measurement of the lower mantle minerals will be attained using this system. More recently, higher pressure ultrasonic measurements of Mg-perovskite have been started, combined with the sintered diamond anvils. In this presentation, the recent experimental results of lower mantle minerals under high pressure will also be present.

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*Speaker

High-pressure single-crystal elasticity measurements of Al-Fe-bridgmanite up to lower mantle pressures

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The chemical composition of the Earth's lower mantle can be constrained by combining seismological observations with mineral physics elasticity measurements. Here, we report single-crystal elasticity data on Al-Fe-bearing bridgmanite using single-crystal high-pressure Brillouin spectroscopy and X-ray diffraction. Two crystals of (Mg0.9Fe0.1Si0.9Al0.1)O3 bridgmanite with different crystallographic orientations were cut using a focused ion beam and were loaded in the pressure chamber of a single diamond anvil cell. Elasticity and density measurements were performed at high-pressures on both samples using a combined Brillouin scattering and X-ray single crystal diffraction system at BGI. Our results show that the Fe/Al substitution in the MgSiO3 structure reduces the acoustic velocities at room pressure. Moreover the compressional wave velocities remain smaller at all pressures, whereas the larger pressure dependence of the shear velocities leads to a shear velocity crossover with MgSiO3 bridgmanite at pressures above 35 GPa. We employ our data to model seismic wave velocities in the top portion of the lower mantle assuming a pyrolitic mantle composition. We find good agreement between our mineral physics predictions and the seismic PREM down to at least 1200 km depth. A high Fe3+/Fe2+ ratio of about 2 in shallow lower mantle bridgmanite is required to match seismic data, implying the presence of metallic iron in an isochemical mantle. Our calculated velocities are in increasingly poor agreement with those of the lower mantle at depths > 1200 km, indicating either a change in bridgmanite cation ordering or a decrease in the ferric iron content of the lower mantle that has potential implications for geochemistry and geophysics.

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*Speaker

Crystal structure of MgO along the shock Hugoniot

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Of the more than 6,000 confirmed and candidate extrasolar planets discovered to date those that are 1-4 times the radius of the Earth are found to be the most abundant. The silicate compounds that dominate the Earth's mantle likely dissociate into component oxides at the extreme pressures (200-2,000 GPa) and temperatures (5,000-10,000 K) corresponding to conditions of super-Earth mantles. Magnesium oxide (periclase), an end-member of the ferropericlase solid solution (Mg,Fe)O and an important component the Earth's mantle, has been studied under static compression in the pressure and temperature range found within the Earth (_˜135 GPa, 2500-4000 K). However, as static compression techniques are typically limited to peak pressures of $<$ 200 GPa, much less is known about its behavior under high-pressure and -temperature conditions. In this study, the structure of MgO upon shock compression over the 200-700 GPa pressure range was examined at the Omega-EP Laser facility at the Laboratory for Laser Energetics, University of Rochester. Laser drives of up to 2 kJ over 10 ns focused onto a polyimide ablator were used to shock compress 50-μm thick polycrystalline or single-crystal MgO. At peak compression, the sample was probed with He-α X-rays from a laser-plasma source. Diffracted X-rays were collected using the PXRDiP diagnostic which consists of image plates lining the inner walls of a box attached to the target package. For each pressure we measure crystal structure, pressure (velocity interferometry), density (x-ray diffraction) and shock temperature (pyrometry). Along the shock Hugoniot MgO transforms from B1 to the B2 structure at _˜400 GPa and

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*Speaker

melts at ~700 GPa. Additional experiments using a decaying shock geometry combined with temperature measurements at the shock front provide a continuous measurement of pressure and temperature changes across the B1-B2 and B2-liquid phase boundaries.

Perspectives for static and dynamic high-pressure experiments at the High Energy Density Science (HED) instrument at European XFEL

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With unique properties, like pulse length, coherence and brilliance, free-electron laser facilities offer new perspectives for the study of matter at extreme conditions. The extremely high brilliance offers the possibility to achieve single shot structural and spectroscopic data of short-lived states. At the upcoming facility of the high energy density science instrument (HED) at the European X-ray Free Electron Laser in Schenefeld, Germany, hard X-rays with energies between 5 and 25 keV, a photon flux of about 10E+12 photons/pulse at 12 keV photon energy, pulse durations from 2 - 100 fs will be available from the SASE2 undulator [1]. Relative bandwidths vary between 10E-3 in FEL mode, or _˜10E-4 in monochromatic or seeded mode.
At HED with important contributions by the international user consortium *Helmholtz International Beamline for Extreme Fields* (HIBEF) [2,3], it will be possible to study materials at temperatures of up to several 1000 K and up to 1 TPa by shock and ramp compression with an optical long pulse laser (DIPOLE100X). The short-lived states can be investigated with several X-ray techniques, such as XRD, XANES and Thomson scattering. In addition, phase contrast imaging will allow visualizing the response of the material by imaging snapshots at the fs timescale. In addition to high-pressure studies using an optical laser, the high photon energies will enable for the first time to use diamond anvil cells at an FEL. Besides a set-up for conventional DACs, which is optimized for XRD, it is planned to build a set-up for dynamic DACs as well as a pulsed-laser heated system.

HED will be an open user instrument with beam distribution based of peer-reviewed scientific proposals [4]. User experiments are planned to start end of 2018.

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[*] Speaker

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[4] see www.xfel.eu

Amorphous and liquid samples structure and density measurements at high pressure – high temperature using diffraction and imaging techniques

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Determination of the density and structure of liquids such as iron alloys, silicates and carbonates is a key to understand deep Earth structure and dynamics. X-ray diffraction provided by large synchrotron facilities gives excellent results as long as the signal scattered from the sample can be isolated from its environment. Different techniques already exist; we present here the implementation and the first results given by the combined angle- and energy-dispersive structural analysis and refinement (CAESAR) technique introduced by Wang et al. in 2004, that has never been used in this context. It has several advantages in the study of liquids: 1/ the standard energy-dispersive technique (EDX), fast and compatible with large multi-anvil presses frames, is used for fast analysis free of signal pollution from the sample environment 2/ limitations of the EDX technique (homogeneity of the sample, low resolution) are irrelevant in the case of liquid signals, others (wrong intensities, escape peaks artifacts, background subtraction) are solved by the CAESAR technique 3/ high Q data (up to 15 A-1 and more) can be obtained in a few hours (usually less than 2). We present here the facilities available on the PSICHE beamline (SOLEIL synchrotron, France) and a few results obtained using a Paris-Edinburgh (PE) press and a 1200 tons load capacity multi-anvil press with a (100) DIA compression module.
X-ray microtomography, used in conjunction with a PE press featuring rotating anvils (RotoPEc, Philippe et al., 2013) is also very effective, by simply measuring the 3D volume of glass or liquid spheres at HPHT, thus providing density. This can be done in conjunction with the CAESAR technique and we illustrate this point. Finally, absorption profiles can be obtained via imaging

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*Speaker

techniques, providing another independent way to measure the density of these materials.

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MSPD beamline for high pressure studies at Alba synchrotron

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The Material Science Powder Diffraction (MSPD) beamline of Alba Synchrotron is dedicated to powder diffraction techniques. The superconducting wiggler generates a tunable photon beam between 8 and 50 keV. The beamline consists of two experimental stations positioned in series: a High Pressure station and a High Resolution/High Throughput powder diffraction station. The monochromatic beam is selected using a fixed exit double crystal monochromator and focused onto the sample using multilayers mirrors in the Kirkpatrick-Baez geometry. This is particularly suited for high pressure studies requiring a very small beam. The focal spot showed a 15x15 μm beam spot diameter at full width half-maximum in the range 20-50 keV.

The experimental enclosure of the HP station is dedicated to diamond anvil cells and consists of two towers of stacked rotation/tilt/translation stages supplied by Huber Diffracktionstechnik. The DAC is mounted on a tower composed, from bottom to top, of an XYZ stage/rotation stage/an XY stage (along the beam and vertical). In order to increase the powder averaging the DAC is rotated over a typical 5-30° range. Before the sample, a collimator and pin-hole aperture ranging from 30-200 μm serve to clean the tale of the beam. All the diffraction images are collected using transmission geometry on a Rayonix SX165 CCD detector. The range of the sample to detector distance is situated between 150 and 500 mm with the diffraction images scanned at 80 μm pixel resolution. The HP diffractometer can mount some attachments depending on needed experimental conditions. Most of the DACs, available for users, can be used at high temperature conditions with resistive heating system (_˜ 1000K) while helium cryocooling is employed for low temperatures (_˜ down to 15K).

The potential of the beamline will be illustrated by various results obtained on many scientific cases: study of phase transitions in orthovanadates, pressure effects in nanocrystalline oxides, thallium phase diagram at high pressure and high temperature, pressure induced helium trapping in molecular solids. Finally, futures developments of the beamline will be presented.

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Posters: Rheological and Transport Properties

Thermal conductivity of pyroxenes at high pressure

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The most accepted petrological assembly for the upper mantle is composed of olivine, orthopyroxene, clinoyroxene and garnet. The most accepted petrological assembly for the upper mantle is to be the peridotitic rock which typically composed of olivine, orthopyroxene, clinoyroxene and garnet. Among these four major mineral phases, the olivine and garnet phases remain the same crystal structure under upper mantle conditions while the clinopyroxene phase is possessing monoclinic system till dissolved into garnet. The Mg-rich opx is the only one phase possessing polymorphism at upper mantle conditions, to a high clinoenstatite (hereafter HP C2/c) at normal (warm) mantle conditions. Most recent high pressure X ray diffraction experiment revealed a new high pressure monoclinic phase with space group $P21/c$ (hereafter HP $P21/c$) over pressure of 10 GPa, room temperature in opx (Dera et al., 2013). Interestingly, across this particular transition, the elastic velocity was shown to be softening.

To understand the Earth's thermal state, the thermal transport properties of mantle phases are desired. In this study, we are interested in thermal conductivity of the pyroxene phases under high pressure and across the phase transition. To carry out such measurement, a technique "Time-domain thermoreflectance" (TDTR) will be employed interfaced with diamond anvil cell to measure the thermal conductivity of orientated single-crystals.

The thermal conductivity of Fe-bearing opx and diopside were obtained in different crystallographic orientations up to 12 GPa. A discontinuity in the thermal conductivity of opx was observed due to the phase transition. In this meeting we present the details of measurements and the comparison with that of olivine phase.

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[*] Speaker

Phonon lifetime of MgO by inelastic x-scattering and ab initio calculations: Implications for thermal conductivity

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Thermal conductivity is a fundamental physical parameter that largely controls the heat transfer in Earth's interior. Despite its importance, the thermal conductivity of mantle minerals is one of the least constrained properties at high pressure (P) and high temperature (T) as direct measurements at pertinent P-T conditions remains a technical challenge. Current geophysical models rely on the extrapolations of low P data and, increasingly so, on results from ab initio calculations. However, the validity and versatility of the various theoretical approaches used in literature remain to be tested again experiments. The direct measurements of vibrational and anharmonic properties such as phonon energy and linewidth as a function of P and T provide the most straightforward benchmark for the theoretical calculations as these are the key parameters entering the Boltzmann transport equation used to calculate lattice thermal conductivity.

Here we present the determination of phonon energies and phonon widths of single crystalline MgO at room temperature and 1220K by inelastic x-ray scattering and by density functional theory. The comparison of experimental and computational results allows assessing the theoretical phonon-phonon scattering coefficients and to estimate the relative weight of intrinsic and extrinsic phonon scattering mechanisms.

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The Androgynous Twins of Zinc

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Zn is a hexagonal metal with a large c/a ratio under ambient conditions (c/a=1.856). Under ambient testing conditions, deformation is predominantly accommodated by basal slip and by {10-12} compression twinning. Increasing hydrostatic pressure drastically reduces the c/a ratio of Zn. As a consequence, the compression twin is predicted to become a tensile twin when c/a $< \sqrt{3}$ at P $>$ 9 GPa.
In this work we strain-cycle a wire of pure Zn in the D-DIA deformation press under multiple superimposed hydrostatic pressures ranging between 3 and 17 GPa. Over this pressure range, the c/a ratio of Zn goes over the compressive-tensile transition. During deformation, the state of the sample is monitored in-situ through powder x-ray diffraction, allowing the extraction of texture and sample stress. Elasto-visco-plastic polycrystal simulations of the cyclic process allow us to interpret the experimental data and to elucidate the type and strength of the crystallographic deformation mechanisms.
The purpose of this work is to elucidate the active deformation modes as a function of pressure. Specifically: 1) to determine if detwinning is a possible mechanism at 3 GPa pressure when Zn is cycled in tension-compression; 2) to find out if at a pressure state where c/a $\sim \sqrt{3}$ only basal slip is active or whether another slip mechanism operates, and which; 3) to find out whether {10-12} tensile twins are active in Zn when c/a $< \sqrt{3}$. This work will help to better constrain the effect of hydrostatic pressure on the plastic deformation of hcp metals.

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Is thermal conductivity of hcp iron anisotropic?

Kenji Ohta *† [1], Yuuki Sato [2], Yu Nishihara [3], Takashi Yagi [4], Kei Hirose [5], Saori Kawaguchi-Imada [6], Naohisa Hirao [6], Yasuo Ohishi [6]

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At some time in the past, the Earth's liquid iron core began to solidify from the inside out, resulting in a growing solid inner core, which has a key role in powering the Earth's dynamo action. The inner core is known to be elastically anisotropic. The cause of the seismic anisotropy in the inner core can be explained by the crystallographic preferred orientation (CPO) of hexagonal closed packed (hcp) iron that is widely believed to be a main component of the inner core. However, it is still unclear how to occur and sustain such CPO of the inner core material although many hypotheses have been proposed. Anisotropy in the thermal conductivity of hcp iron may have important implications for the structure and thermal evolution of the Earth's inner core (Secco and Balog, 2001 *Can. J. Earth Sci.*). However, the conductivity anisotropy in hcp iron has never been examined partly because the hcp phase of iron is stable above 13 GPa and unquenchable to ambient conditions. In this study, we investigated anisotropy in thermal conductivity of hcp iron to 35 GPa based on synchrotron X-ray diffraction measurements and the pulsed light heating thermoreflectance technique in a diamond anvil cell. We found that the thermal conductivity of hcp iron along c axis is about twice larger than that along a axis at 35 GPa. Such anisotropic thermal conductivity in hcp iron could sustain crystal alignment in the inner core that causes seismic anisotropy. In addition, the anisotropic conductivity in hcp iron may resolve the problem in the conductivity of iron at the core conditions (Ohta et al., 2016 *Nature*; Konôpková et al., 2016 *Nature*; Dobson, 2016 *Nature*).

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Compositional and Pressure-Temperature dependence of the thermal conductivity of bridgmanite

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The amount of heat flow from the Earth's core to mantle critically determines the thermo-chemical evolution both of the core and the mantle. Bridgmanite, iron and aluminum bearing MgSiO3 perovskite, is the most abundant mineral in the Earth's lower mantle, and thus its thermal transport property mainly controls heat transport in the lower mantle. Here we measured lattice thermal diffusivity of bridgmanite with 5 different chemical composition up to 180 GPa at ambient temperature, and also at high temperature up to 600 K using the pulsed light heating thermoreflectance technique in a diamond anvil cell. Our results indicate that the lattice thermal conductivity of the bridgmanite sample is slightly lower than that of iron and aluminum free bridgmanite determined by using the same experimental technique (Ohta et al., 2012) and ab initio calculation (Dekura et al., 2013). Our results exhibit moderate effect of iron and aluminum incorporation into bridgmanite on its thermal conductivity, which imply temperature variation in the lower mantle tends to easily induce heterogeneity of thermal conductivity and core heat flux there that could drive large scale dynamics both in the core and mantle.

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*Speaker

Effect of Fe content on olivine strength at high-pressure and comparison with ringwoodite

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Terrestrial planet mantles are olivine-rich, with Fe/(Mg+Fe) ratio lower than _˜2% for Mercury and up to 25-30% for Mars, with intermediate compositions for the Earth and Venus. Experiments at 300 MPa pressure (Zhao et al., 2009, EPSL, 287, 229-240) indicate that Fe dramatically decreases olivine viscosity. Thus, the Martian upper mantle may be _˜10 times less viscous than the Earth's at the same conditions. Whether such a weakening occurs at the high pressures relevant to planetary interior is unknown. Deeper in the mantle, olivine (α) transformed into its high-pressure polymorphs wadsleyite (β) and ringwoodite (γ), the main constituents of the transition zone. Understanding the strength contrast between olivine and or phase is critical to constrain mantle convection. Here, we present the results of a series of high-temperature deformation experiments carried out in the D-DIA coupled with synchrotron radiation at pressure (P) within 1.5 – 6.5 GPa, on polycrystalline olivine specimens with various compositions along the forsterite - fayalite joint. Specimens and cell assembly were kept dry at 120°C for several hours before loading into the D-DIA. Different specimens were deformed two by two in order to compare their rheology, while San Carlos olivine was used as a reference material. In a few preliminary experiments, Fe-rich γ phase rheology was compared with that of Fe-poor olivine. We will show that pressure dramatically decreases the viscosity contrast between Fe-poor olivine and Fe-rich olivine, while increasing differential stress has the opposite effect. Hence, the range of viscosities expected in planetary mantles - between the low-P high-stress regime of the subsurface and the high-P low-stress regime of the deep interior – may strongly depends on their iron contents. We will also discuss the viscosity contrast between olivine and its high-pressure polymorphs as observed in our preliminary experiments, in the framework of previously published data.

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[*] Speaker

Laboratory constraints on the mechanism of deep crustal earthquakes under southern Tibet

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Deep crustal earthquakes under Southern Tibet occur to depths of ˜ 100 km, within the subducted Indian continental plate, where the lower crust is considered hot and dry [Hacker et al., Science, 2000]. Such seismicity cannot be produced by simple brittle shear fracture or frictional sliding, because of the high pressure conditions. Pseudotachylytes, "fossilized" fault zones of past earthquakes, were found in western Norway under conditions corresponding to the eclogite facies stability field [Austrheim & Boundy, Science, 1994], suggesting that eclogitization is potentially involved in deep crustal seismicity: faulting took place in metastable granulite (the main constituent of lower continental crust) at pressures approaching ˜3 GPa (i.e., depths of 100 km), inducing melting in the fault zone that crystalized into pseudotachylites. Here we conduct deformation experiments on natural and nominally dry granulite in a deformation-DIA (DDIA) apparatus within the stability fields of both granulite and eclogite. The D-DIA, installed at beamline 13-BM-D of GSECARS at the Advanced Photon Source, is interfaced with an acoustic emission (AE) monitoring system, allowing in-situ detection of mechanical instability along with the progress of eclogitization (by x-ray diffraction). We found that granulite deformed within its own stability field ($<$ 2 GPa and 1000○C) behaved in a ductile fashion without any AE activity. In contrast, numerous AE events were observed during deformation of metastable granulite in the eclogite field above 2 GPa. Correlating closely with AE burst episodes, measured differential stresses rose and fell during deformation, suggesting unstable fault slip. Microstructural observation on recovered samples shows that strain is localized around grain boundaries, which are decorated by eclogitization products. Cavitation along the grain boundaries suggests significant grain boundary sliding. Thus, metastable dry granulite fails by grain boundary weakening. Ruptures originate from weakened grain boundaries, propagate through grains, and self-organize into macroscopic fault zones. No melting is required in the fault zones to facilitate brittle failure. This process may be responsible for the deep crustal seismicity in Southern Tibet and other continental-continental subduction regions.

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Deformation of bridgmanite and post-spinel two-layered sample under lower mantle conditions with DT-Cup apparatus

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Viscosity jump at 800- to 1200-kilometers depth was reported by geophysical observation recently (Rudolph et al., 2015). Due to the absence of phase transition in the main minerals, chemical deviation is one candidate explanation for the viscosity jump. A perovskitic lower mantle is consist of more than 93 vol.% bridgmanite (Murakami et al., 2012), on the other hand, subducted harzburgite layer contains ˜20 vol.% of ferropericlase (Irifune and Ringwood, 1987). Ferropericlase is likely much weaker than bridgmanite may significantly reduce the bulk viscosity of bridgmanite and ferropericlase aggregate (Yamazaki and Karato, 2001). Therefore, the viscosity of bridgmanite and ferropericlase aggregate is critical for us to understand the viscosity profile in the lower mantle.

To identify the bulk viscosity of bridgmanite and ferropericlase aggregate, two-layered sample of bridgmanite and post-spinel (bridgmanite plus ˜ 30 vol.% of ferropericlase) aggregates were deformed simultaneously. We prepared starting material of bridgmanite and post-spinel aggregates with grain size of 5-10 um at high pressure and high temperature in a Kawai-type high-pressure apparatus. Then the deformation experiments were conducted in the DT-Cup apparatus which is a development of the Kawai type multi-anvil press (Hunt et al., 2014).We deformed bridgmanite and post-spinel two-layered samples up to strain of ˜0.2 at 1500 ◦C and 25 GPa. As the identical uni-axial stress during deformation, the strengths of bridgmanite and post-spinel are inversely proportional to their strains.

The recovered bridgmanite and post-spinel samples showed virtually identical strain, which indicates similar strengths of them. Lattice preferred orientations (LPOs) of bridgmanite phase in both bridgmanite and post-spinel samples are similar developed, the slip plane of (100) is consistent with the slip system reported by Tsujino et al. (2016). Our result indicates chemical deviation in ferropericlase proportion is unable to be responsible for the viscosity jump in the lower mantle under current condition. The discordance between this study and Girard et al. (2016), who reported a marked softening of post-spinel aggregate with shear strain up to 1.0, highlights the possible importance of large shear strain in controlling the bulk viscosity.

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*Speaker

Posters: Elastic and Structural Properties

High-pressure high-temperature single-crystal elasticity of iron-bearing wadsleyite: Reappraising the water sensitivity of seismic observables

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The Earth's deep water cycle carries hydrogen into the mantle by subduction processes entailing the potential formation of deep hydrogen reservoirs throughout Earth's history. At depths between 410 km and 660 km, large amounts of water can be stored by the nominally anhydrous minerals wadsleyite and ringwoodite. Low seismic velocities are commonly accepted as an indicator for hydration as suggested by previous mineral physics experiments. The detection of hydrated regions within the transition zone by seismology, however, led to contradicting results. We present simultaneous sound wave velocity and density measurements on iron-bearing wadsleyite single crystals at high pressures supplemented by first experiments at combined high pressures and high temperatures. Direct comparison of our results with earlier work shows that both P-wave and S-wave velocities of anhydrous and hydrous iron-bearing wadsleyite converge at high pressure to become seismically indistinguishable at conditions of the transition zone. As a consequence, seismic tomography might be unsuitable to map water in the shallow transition zone. We further modelled velocity, density, and acoustic impedance contrasts across the 410-km seismic discontinuity and found that velocity contrasts change only slightly on hydration. Instead, our results suggest that impedance contrasts are more sensitive to hydration and hence that the reflectivity of the 410-km discontinuity might serve as a more reliable indicator for water in the transition zone.

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Elastic properties of fayalite

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Olivine, a solid-solution between forsterite (Mg2SiO4) and fayalite (Fe2SiO4) is one of the most abundant minerals in the mantles of terrestrial planets. The knowledge of its thermo-elastic parameters is essential to understand and model planetary interiors. Because the accepted average composition of Earth's mantle olivines is around [Fe0.1,Mg0.9]2SiO4, Mg-rich olivines have been extensively studied. In comparison Fe-rich olivines have received little attention. We performed a series of experiments in orde to measure equations of state of olivines with compositions ranging from [Fe0.4,Mg0.6]2SiO4 to Fe2SiO4. The purpose is to better constrain the effect of Fe content on elastic properties of olivines. We will mostly present our results obtained on fayalite Fe2SiO4.

Our fayalite samples were synthesized from nano-size powders of elementary oxides mixed with the proper stoichiometries and reacted at room pressure and 1000◦C under controlled atmosphere. The fully reacted powders were then sintered using Spark Plasma Sintering in order to minimize the porosity of our samples. The resulting olivine aggregates have homogeneous grain sizes, close to 2 μm. High-pressure high-temperature experiments (up to about 7 GPa and 600◦C) coupled with synchrotron X-ray diffraction and X-radiographic imaging were conducted using the DIA apparatus at the X17B2 beamline at NSLS (Brookhaven, N.Y., U.S.A). This setup allowed us to estimate the deviatoric stress present in both the sample and NaCl, the pressure calibrant. We also performed ultrasonic interferometry measurements in order to obtain P- and S-wave travel times using the DIASCoPE setup at X17B2. The sample density was determined in situ using X-ray diffraction, the sample length was measured under extreme conditions using the X-radiographic image, and the acoustic travel times were measured using the ultrasonic interferometer. The travel times combined with sample lengths yield the P- and S-wave velocities in the sample, and these data combined with the density gives a direct measurement of the elastic bulk and shear moduli under all conditions of the experiment.

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Our presentation will focus on results obtained on Fe2SiO4 samples from X-ray diffraction and ultrasonics experiments, in particular the role of the deviatoric stress on the elastic properties will be discussed.

Velocity-Density Systematics in Fe-Si Alloys at Extreme Conditions

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Physical properties and dynamics of the Earth's core are critically dependent on the chemical composition. As there is no direct method for sampling core materials, compositional models are obtained by comparing seismological observations to profiles of density, compressional sound velocity (Vp) and shear velocity (Vs) of candidate alloys as a function of pressure. So far, most of the experimental studies have been limited to the measurement of end-members or commercially-available alloys with light-element contents much larger than what would be expected in the Earth's core. Proposed compositional models of the core are then based on a linear interpolation (linear-mixing approximation) to a more realistic inner core composition. Here we present Vp and density measurements of solid Fe-Si alloys compressed under quasi-hydrostatic conditions to megabar pressures by combined picosecond acoustics and synchrotron X-ray diffraction. By systematically varying alloy composition, we present Birch diagrams of a range of bcc and hcp iron-silicon alloys and discuss the validity of linear-mixing models for this system.

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*Speaker

Sound velocities of CaSiO3 perovskite

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Laboratory measurements of sound velocities of high-pressure minerals provide crucial information on the composition and constitution of the deep mantle via comparisons with observed seismic velocities. CaSiO3 perovskite (CaPv) is considered to be a major high-pressure phase at depths greater than _˜560 km in the mantle and the subducting oceanic crust. On the basis of experimental data on the elastic properties of tetragonal CaPv, previous studies have argued that variation in the abundance of CaPv in the mantle could explain high shear to longitudinal wave velocity heterogeneities in the deep mantle. At the P and T of the mantle however, CaPv adopts a cubic structure above _˜600 K but despite its importance, measurements of sound velocity of the cubic CaPv under the corresponding P, T conditions has never been performed because this phase is unquenchable to atmospheric pressure and adequate samples for such measurements are unavailable. Here we report *in situ* X-ray diffraction and ultrasonic sound velocity measurements up to 23 GPa and 1700K (equivalent to the depths of the bottom of mantle transition region) using a high-density CaSiO3 glass rod specimen, that is first converted to a sintered polycrystalline body of cubic CaPv under high pressure and temperature in a multianvil apparatus. We observed a sudden change in sound velocities around _˜650K, consistent with the temperatures of the cubic to tetragonal transition in CaPv, thereby obtaining the elastic properties of both of these perovskites independently. We found cubic CaPv, which is more likely to be relevant to the mineralogy of the mantle, has a shear modulus _˜26% lower than theoretical predictions, implying that either pyrolite or basaltic compositions yield too low seismic velocities and fail to explain the observed velocities in the lower half of the mantle transition region. The existence of the former basaltic crust below the 660 km depth underneath some subduction zones may however explain the low shear-velocity region observed atop of the lower mantle.

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*Speaker

Thermoelastic properties of Al-bearing hydrous bridgmanite

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Water is the most abundant volatile component on the Earth. It has significant influences on the chemical and physical properties of mantle minerals (e.g., melting temperature, elastic properties, electrical conductivity, and so on.). Recently, hydrous ringwoodite contained _˜1.5 wt% water was discovered by Pearson et al. (2014) as an inclusion in ultra-deep diamond. This observation implies that the mantle transition zone contains some water at least locally. On the other hand, water solubility of bridgmanite which is the most abundant mineral in the lower mantle, is a matter of debate (e.g., Bolfan-Casanova et al., 2000). In this situation, Al-bearing hydrous bridgmanite contained _˜0.8 wt % water was synthesized by Inoue et al. (in prep). However, the physical properties of Al-bearing hydrous bridgmanite under high pressure and high temperature has not been clarified yet. In this study, we clarified P-V-T equation of state of Al-bearing hydrous bridgmanite.

We conducted the room temperature compression experiments using diamond anvil cell with He pressure medium up to _˜55 GPa under quasi-hydrostatic condition (Takemura, 2001) at KEK PF BL18C. The compression data of Al-bearing hydrous bridgmanite was obtained at room temperature. In addition, the P-V-T experiments using multi-anvil high pressure apparatus with sintered diamond 2nd stage anvil at SPring-8 BL04B1 were performed. The in situ closed system experimental method using Ag capsule was developed for preventing the dehydration of Al-bearing hydrous bridgmanite.

The bulk modulus of Al-bearing hydrous bridgmanite was found to be much smaller than that of Mg-endmember bridgmanite (Tange et al. 2012). On the other hand, thermal expansion was larger than that of Mg-endmember bridgmanite. By comparing our obtained results with PREM, we will discuss the possible water content in the lower mantle.

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[*] Speaker

Sound velocities and elastic constants of single crystal Pt under high pressure

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Recently high pressure experimental techniques using a diamond anvil cell (DAC) have progressed and the phase relationships under the pressure conditions corresponding to the center of the Earth have been investigated (e.g. Tateno et al., 2010). The experimental pressures were generally decided based on an equation of state of a pressure scale (EOS). The EOSs were usually determined based on different pressure scale, such as Au, Pt, and NaCl. For instance, the pressure at the ICB condition of Holmes scale is approximately 10% higher than that of Fei scale (e.g. Fei et al., 2007; Holmes et al., 1989). Therefore, EOSs of a sample may give different pressures if the EOSs are established based on different EOSs of same pressure scale. It is important to determine the EOS independently from other scales. Measuring volumes or densities with sound velocities enables us to establish an independent EOS. Therefore, we have measured sound velocities of a single crystal of Pt under high pressure based on inelastic X-ray scattering and its volumes were simultaneously measured. The Pt single crystal was commercially purchased from MaTeck Co. A small piece of the single crystal of Pt was cut by FIB. The culet size used here was 400 μm. The small piece of single crystal of Pt was set in the sample chamber with ruby tips. Before loading Helium gas as a pressure medium inelastic X-ray scattering measurements were performed at room temperature and ambient pressure. The crystal parameter, $a0$, was also measured before the IXS measurements. The reference pressures were measured before and after each IXS measurement and crystal parameter, a, was measured before each IXS measurement. The sound velocities of single crystal of Pt were measured at 0, 1, 6, 10, 15, and 21 GPa. Cijs at ambient pressure were obtained to be C11=306(1), C12=193(1), and C44=56.4(2) GPa and C11=332(3), C12=228(3), and C44=62.8(3) GPa were obtained for 1 GPa. These values are slightly smaller than previous studies (Macfarlane et al., 1965; Menendez-Proupin and Singh, 2007). We will discuss the Cijs and EOS based on our results.

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Compressibility of MgCO3 phase II under the lowermost mantle conditions

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MgCO3 magnesite is one of the important carbonate minerals in the deep Earth because it can be a carbon carrier from the surface to the mantle with subducted slabs (e.g., Dasgupta and Hirschmann, 2010). The significant observation is phase transitions of MgCO3 from magnesite to high-pressure phases under the lower mantle conditions (e.g., Isshiki et al., 2004; Oganov et al., 2008). Several recent studies have supported a monoclinic MgCO3 (”phase II”) as a post-magnesite phase composed of (C3O9)-ring units above 80 GPa (e.g., Oganov et al., 2008; Boulard et al., 2011). However, the physical and chemical properties of MgCO3 phase II have not been revealed yet. Such information is required to understand contribution of MgCO3 to the Earth's carbon cycle. We have investigated the compressibility of MgCO3 phase II up to the lowermost mantle conditions.

A starting material was a natural magnesite (Mg0.997Ca0.003CO3) from Bahia in Brazil. Experimental conditions up to 145 GPa and 2900 K were generated using a double-sided laser-heated diamond anvil cell. Culet diameters of diamond anvils used were between 100 and 250 μm. The sample was loaded into a sample chamber in a tungsten gasket which was pre-indented to 40–60 μm in thickness and drilled a 60–80-μm hole in diameter. Laser heating was conducted using a fiber laser absorbed by Pt or Au which served as a pressure scale. Run products were investigated using synchrotron X-ray diffraction (XRD) at BL10XU of SPring-8 in Hyogo, Japan. Experimental pressures were measured using a thermal equation of state (EOS) of Pt or Au (Fei et al., 2007).

We observed the monoclinic phase II having space group C2/m (Oganov et al., 2008) above 85 GPa after laser heating. The unit cell volume of phase II is obtained by fitting the XRD patterns. The present results with the data in Maeda et al. (2017) were fitted by the second-order Birch-Murnaghan EOS to acquire the bulk modulus K0T = 210.7 (2) GPa and unit cell volume V0 = 469.8 (2) Å3 at room temperature. Density increase from magnesite to phase II can be 6–9 % above 85 GPa. The present results shows some difference with the previous calculation (K0T = 156.76 GPa, V0 = 503.36 Å3 and K'0T = 4.12 at 0 K; Oganov et al., 2008).

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Single-Crystal Elastic Constants of Forsterite as a Function of Pressure and Temperature Simultaneously to 0.5GPa and 773K: Geophysical Implications for the Upper Mantle

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Employing high precision ultrasonic interferometry techniques, we have measured the 9 single-crystal elastic constants Cij of pure forsterite, via 18 velocity modes, as a function of pressure (to 0.5 GPa) and temperature (to 773 K). The values of Cij, $(\partial Cij/\partial P)$ at ambient temperature, and $(\partial Cij/\partial T)$ at ambient pressure are in good agreement with those reported previously by Kumazawa and Anderson (1969), and Graham and Barsch (1969). We have found that the values of $(\partial Cij/\partial P)$ increase with increasing temperature; the temperature effect is more profound for the longitudinal moduli (especially C11) as compared to that for shear moduli. We have also measured, for the first time, the temperature dependence of the pressure derivatives of all the 9 Cij to 573 K, providing the values of $(\partial^2 Cij/\partial P\partial T)$T,P. Although the pressure and temperature ranges of our data are limited, the high degree of accuracy of these techniques and the resolution of cross-derivatives allows extremely accurate extrapolation of the properties of olivine throughout its stability field. In particular, measurements of these cross-derivatives of the elastic moduli are deployed to assess the velocity anisotropy of olivine as a function of pressure and temperature, and thus to more accurately calculate the degree of alignment necessary to generate seismically-observed mantle anisotropy as a function of depth in different thermal environments: such constraints on preferred orientation are of fundamental importance in determining the flow field in the upper mantle, and associated with surface tectonics. Furthermore, such data can be utilized to accurately constrain the density of olivine at its highest pressure/temperature equilibrium occurrence in the mantle–directly above its transition to the wadsleyite phase near 410 km depth. Thus, these data, in tandem with accurate wadsleyite data, can illustrate what density jump is anticipated for (Mg,Fe)2SiO4 across this mantle transition.

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*Speaker

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Measurements of Elastic and Inelastic Properties of Polycrystalline Samples under Simulated Earth's Mantle Conditions in Large Volume Apparatus

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The interpretation of highly resolved seismic data from Earth=s deep interior require measurements of the physical properties of Earth's materials under experimental simulated mantle conditions. More than a decade ago seismic tomography clearly showed subduction of crustal material can reach the core mantle boundary under specific circumstances. Considering this geophysical high pressure research is faced the challenge to increase pressure and sample volume at the same time to be able to perform in situ experiments with geophysical representative complex samples. Recent large volume presses at synchrotrons provide sample volumes 3 to 7 orders of magnitude bigger than in diamond anvil cells far beyond transition zone conditions. The sample size of several cubic millimeters allows elastic wave frequencies in the low to medium MHz range. Together with the small and even adjustable temperature gradients over the whole sample this technique makes anisotropy and grain boundary effects in complex systems accessible for elastic and inelastic properties measurements in principle. The real elastic wave propagation have also no limits for opaque and encapsulated samples. Using triple-mode transducers and the data transfer function technique for ultrasonic interferometry makes transient measurements in complex systems under non-equilibrium conditions possible. Ultrasonic interferometry necessarily requires in situ sample deformation measurement by X-radiography. In situ falling sphere viscosimetry require time-resolved X-radiography. Using a D-DIA even the measurement of elastic and inelastic properties in the seismic frequency range is achievable. The paper presents techniques and results of recent experimental high pressure geophysics in LVPs.

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*Speaker

Variable-temperature single-crystal X-ray diffraction study of SrGeO3 high-pressure perovskite phase

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The high-pressure cubic perovskite phase of SrGeO3 is earth-scientifically important as a potentially good low-pressure analog of CaSiO3 cubic perovskite, a constituent mineral in Earth's lower mantle. Despite such importance, only a few structural studies of SrGeO3 perovskite have been reported. Investigations for temperature dependence of crystal structure, such as thermal expansion and atomic thermal vibration behavior, provide insights into interatomic interaction, and hence are dispensable for the understanding of the structure stability. We here conduct single-crystal X-ray diffraction study of SrGeO3 perovskite at different temperatures.

Single crystals of SrGeO3 perovskite were grown at 6 GPa and 1223 K using a 700 ton cubic anvil-type press. Single-crystal X-ray diffraction experiments were conducted over the temperature range of 100 to 473 K. The experiments showed that the crystal begins to deteriorate at a higher temperature than 323 K and completely amorphizes by 448 K. The structure refinements were therefore performed at seven temperature-points in the range of 100 to 323 K.

The thermal vibration of the O atom is remarkably anisotropic and its displacement ellipsoid is considerably suppressed in the direction of the Ge-O bond. The mean square displacement (MSD) of the O atom in the direction of the Ge-O bond is almost temperature-independent, whereas that in the direction perpendicular to the bond largely increases with increasing temperature. This peculiar thermal vibration behavior of the O atom can be due to a strong covalency of the Ge-O bond. This conclusion is led from the following results: (1) the degree of covalency in the Ge-O bond evaluated from the bond valence, (2) the observation of the residual electron density peaks originating in the bonding electrons of the Ge-O bonds and (3) the large one particle potential coefficients of Ge atom evaluated from Debye temperatures determined by the Debye model fitting to the temperature dependence of MSD.

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*Speaker

Compressional behavior of δ-(Al, Fe)OOH to lower mantle pressures

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Delta-AlOOH is an important hydrous mineral for understanding the water cycle in the deep Earth. In a hydrous slab penetrating Earth's lower mantle, δ-AlOOH forms a solid solution with Phase H (MgSiO4H2) and ϵ-FeOOH (e.g., Ohtani et al., 2001; Nishi et al., 2015; Ohira et al., 2014). This phase may modulate Earth's deep water cycle, influencing the dynamics and the travel times of seismic waves in the lower mantle. However, the elasticity and related properties of this phase have not been constrained.

In this contribution, we report the behavior of δ-(Al, Fe)OOH at high pressures. The P-V profiles of polycrystalline δ-(Al0.95, 57Fe0.05)OOH (AF5) and δ-(Al0.88, 57Fe0.12)OOH (AF12) (Kawazoe et al., 2017) were measured using X-ray diffraction up to 65 GPa using a membrane diamond anvil cell at BL10XU, SPring-8. The Debye sound velocity (*vD*), Lamb-M´ossbauer factor (*fLM*), and the spin state were determined using nuclear resonant inelastic X-ray scattering and synchrotron M´ossbauer spectroscopy at sector 3, Advanced Photon Source.

A change in the compressibility was observed in the P-V data of AF5 and AF12 at 10-12 GPa, which is in the vicinity of a $P21nm$ to $Pnnm$ structural transition. At similar pressures, *fLM* and *vD* exhibit minimum values. We interpret this *softening* to be related to the onset of proton tunneling that is suggested in pure δ-AlOOH (Sano-Furukawa et al., 2009; Kuribayashi et al., 2014; Bronstein et al., 2017). However, the significant depression of sound velocity was observed only in δ-(Al, Fe)OOH, not in the pure Al-endmember δ phase (Mashino et al., 2016), thus the incorporation of Fe has the potential to enhance the softening of this phase. With increasing pressure, another change in the compressibility was observed, which may be caused by the high-spin (HS) / low-spin (LS) transition of Fe3+ in the δ phase. We will discuss the implications of our results for Earth's lower mantle.

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Vibrational Spectroscopy of Laser Shocked PMMA

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An understanding of material behavior under shock compression is important for variety of applications such as study of material dynamics and chemical reactions. Also, the insight into the pressure, volume and temperature of the materials under shock compression are important. Particularly, in deriving the equation of state of the materials and predicting materials response under extreme temperature and pressure conditions.

Several studies on polymethyl methacrylate (PMMA) under static pressure using Diamond Anvil Cell (DAC) has been carried out. However, the literature on response of PMMA under shock compression still has to be elaborate. The objective of this paper is to understand the response of PMMA under shock compression at molecular level using a pump probe experimental set up. The experiments were performed on confined geometry target assembly by pump and probe technique using high power pulsed laser. The target assembly consists of a cover glass (100×100×5 mm3), a PMMA film sheet (200μm thick), an aluminum foil (50μm thick) and a back-up glass (100×100×5 mm3). The time resolved studies of shock affected region were done by providing delay between pump and probe beam.

The pressure responses of the C-H stretching modes of PMMA in the range 0 to 1.94 GPa range were analyzed. The C-H stretching mode of PMMA observed in this study show inhomogeneous broadening, shift to higher frequency and decrease in intensity with pressure. To estimate the maximum shift under shock compression, it is needed to decompose the Raman spectra and calculate the pressure induced Raman blue shift. The obtained spectra under shock compression are analyzed by fitting double Gaussian peaks.

Both of the observed modes i.e. at 2954 and 2977 cm-1 show increase in the Raman shift with pressure. These shock compressed states are also compared with the static compression data, to see if any general trend can be established. All observed results indicate that the PMMA is stable for the present experimental conditions, with no phase changes or degradation under shock compression. The results of this type are very helpful for benchmarking the theoretical model of materials under high amplitude shock wave compression.

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[*] Speaker

Elastic wave velocities of Fe- and Al-bearing akimotoite by means of ultrasonic measurements

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The Earth's transition zone between 410 and 660 km depth marks a region of transitional seismic wave velocities that increase rapidly with depth between the upper and lower mantle. Models for the mineralogy at the base of the transition zone, using a peridotitic mantle bulk composition, propose the stability of ringwoodite and majoritic garnet. However, by using the elastic properties of these two minerals to estimate the seismic wave velocities, the resulting longitudinal and shear wave velocities are much lower than those actually observed globally for this region. Larger wave velocities may be obtained if the temperatures at the base of the transition zone were lower than expected due to the presence of stagnating cold slab material. Lower temperatures, however, imply the possible presence of akimotoite, a MgSiO3 polymorph stable between 22 and 24 GPa and 1100 to 1700 ◦C. The elastic properties of the MgSiO3 endmember recently have been studied, however, no data are available for compositions relevant for the Earth's transition zone, i.e. containing some Fe and Al substitution. If it can be demonstrated that assemblages containing akimotoite reproduce the transition zone velocity structure, then this would have important implications for the thermal structure and consequently for the dynamics of the Earth's mantle. Three well-sintered polycrystalline akimotoite samples containing 10 mol% of Fe, 20 and 25 mol% of Al were synthesized in a multianvil apparatus at 25 to 27 GPa and 850 ◦C from glassy starting materials. All samples were double-sided polished and inserted into a modified 10/4 multianvil cell assembly equipped with a Re heater and a D-type thermocouple suitable to perform ultrasonic measurements. High pressure and temperature experiments were performed at 13 ID-D (APS) using an ultrasonic system to collect longitudinal and shear wave velocities of the different akimotoite compositions at different pressure and temperature points up to the actual stability conditions of akimotoite of 25 GPa and 1200 ◦C. Synchrotron radiation has been used to measure the exact sample length in-situ employing X-ray tomography and to determine the density of the akimotoite samples. The effect of Fe and Al substitution on the wave velocities of akimotoite will be discussed and compared to seismic reference models.

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*Speaker

Inter-comparison of the Au, Pt and MgO Pressure Scales up to 140 GPa and 2500 K

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Reliable and accurate pressure scales are essential in high pressure research. Because the equations of state (EOSs) of Au, Pt and MgO have been widely used for pressure determination, extensive efforts have been made to improve these pressure scales. However, significant discrepancies still exist among these pressure standards. We measured the unit-cell volume of Pt, Au, and MgO in the mixture of Pt+MgO and Au+MgO in laser-heated diamond-anvil cell up to 140 GPa at both room and high temperatures up to 2500 K. The samples were loaded in either an Ar or Ne pressure transmitting medium. We did not mix Au and Pt together, to avoid alloying at high temperature. The in-situ X-ray synchrotron experiments were carried out at beamlines 13-IDD (GSECARS) and 16-IDB (HPCAT), APS. For the unit-cell volume measured at 300 K after laser heating, we found agreement between the pressure standards within ±2.5 GPa up to 130 GPa. We further refined the EOSs of the three pressure standards at 300 K, making them consistent with each other within ±1 GPa up to 130 GPa ($K0$'= 5.23(3) & $K0$ = 277.3 GPa for Pt; $K0$' = 5.90(2) & $K0$ = 167 GPa for Au; $K0$' = 4.18(2) & $K0$ = 160.3 GPa for MgO). At high temperatures, these three standards agree with each other the best within ±1 GPa between 40 and 140 GPa, adopting the scales by *Dorogokupets and Dewaele* [2007]. However, a 2–3 GPa of discrepancy remains at 20–40 GPa and 1500–2000 K, with gold yielding the highest pressure regardless of pressure scales used. The pressure discrepancy is likely related to steep decreases in the Gr´uneisen parameter, the anharmonicity, and/or the electronic effects for the EOSs of the standards at low pressures (0–40GPa) and high temperature (2000–2500K). Because gold melts near 2000 K at the lower pressure range, severe anharmonic effects expected at pre-melting conditions make the quasi-harmonic EOSs of Au unsuitable for pressure determination at the conditions. Although the pressure scales by *Dorogokupets and Dewaele* [2007] do not completely resolve the discrepancies in the mantle phase boundary properties, they provide tighter constrains on the Clapeyron slopes of the post-spinel boundary to -2.0_˜-2.7 MPa/K and the post-perovskite boundary to 7_˜10 MPa/K. Our data and refined EOSs allow for reliable comparisons among experiments with different pressure standards for the entire P-T conditions expected for the Earth's lower mantle.

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*Speaker

Combined Laser Ultrasonics, Laser Heating and Raman Scattering in Diamond Anvil Cell System

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There is widespread interest in the elastic properties of solids at elevated temperatures and high pressures. Much of the impetus for current research in this area has arisen from geophysical and geochemical studies of the Earth's mantle and core.
Laser ultrasonics (LU) combined with a diamond anvil cell (DAC) has been demonstrated to be an appropriate technique to directly determine the acoustical properties of solids under high pressure. In this report, we describe the development of a multi-functional system for high pressure, high temperature measurements. The system is equipped with a LU set up, Raman device, and laser heating system (LU-LH). Laser ultrasonics combined with LH in a diamond anvil cell (LU-LH-DAC) demonstrated to be an appropriate technique for direct determination of the acoustical properties of solids under high pressure and high temperatures. The use of lasers generating nanosecond acoustical pulses in solids allows measurements of the velocities of shear and longitudinal waves in iron up to 50 GPa. The system is unique and allows us to: (a) measure shear and longitudinal velocities of non-transparent materials under high pressure and high temperature (HPHT); (b) measure temperature in a DAC under HPHT conditions using Planck's law; (c) measure pressure in a DAC using a Raman signal; and (d) measure acoustical properties of small flat specimens removed from the DAC after HPHT treatment.

We present results on measurements of shear and longitudinal wave velocities in iron under high pressure up to 52 GPa, and of the behavior of the velocity of a Rayleigh wave in a PtRh alloy at high temperatures up to 1500 K. Finally, we demonstrate, for the first time, that the LU-LH-DAC technique allows measurements of velocities of the skimming waves in iron at 2580 K and 22 GPa. The ability to detect an LU signal at 2600 K was an unexpected surprise. The maximum intensity of the black body radiation at 2600 K is around 1.1 micron. This is very close to the wavelength of the pump laser (1.06 micron) used for the excitation of the acoustical waves in iron. Therefore, excitation and detection of the acoustical waves by the laser ultrasonics technique is possible even for very bright objects.

Acknowledgments:

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Posters: Melting, Melts and Partial Melts

Iron Partitioning in the Deep Mantle and Consequences for the Magma Ocean

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The relative buoyancy of crystals and liquid is likely to exert a strong influence on the thermal and chemical evolution of the magma ocean. Theory indicates that liquids approach, but do not exceed the density of iso-chemical crystals in the deep mantle. The partitioning of heavy elements, such as Fe, is therefore likely to control whether crystals sink or float. While some experimental results exist, our knowledge of silicate liquid-crystal element partitioning is still limited in the deep mantle. We have developed a method for computing the Mg-Fe partitioning in such systems. We focused initially on (Mg,Fe)O. As a relatively simple system, the buoyancy effects of Fe partitioning are likely to be large. The method is based on molecular dynamics driven by density functional theory (spin polarized, PBEsol+U). We compute the free energy of Mg for Fe substitution in simulations of liquid and B1 crystalline phases via adiabatic switching. With the method tested fully on ferropericlase we then moved to the silicate perovskite system, (Mg,Fe)SiO3. We investigate the dependence of partitioning on pressure, temperature, and iron concentration. In the case of ferropericlase we find that the liquid becomes more dense than the crystal when the pressure increases beyond 40GPa. We also find that the high-spin to low-spin transition in the crystal and the liquid have an important influence on partitioning behavior.

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*Speaker

Dehydration melting of amphibole bearing gneiss and its implication for the high conductivity anomalies in the mid-lower crust of Tibet Plateau

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Magnetotelluric (MT) surveys in the past decades have revealed that high-conductivity layers (0.1-1 S/m) widely exist in the mid-lower crust of Tibet plateau (Wei et al., 2001). In addition, a number of geophysical data sets indicate that these regions are usually characterized by the feature of low velocity (Unsworth et al., 2005). It is of significance to interpret the origin of these low-velocity-high-conductivity zones (LV-HCZs) in the Tibetan crust. Nevertheless, the possible origin is a long-standing and controversial issue.

In this study we investigate the electrical conductivity of amphibolite with different volume fraction of garnet (3 vol% and 18 vol%) at 1.8 GPa and 500-1525 K using an 1260 impedance spectroscopy analyzer. Fast decrease of the sample's resistance from 1250 K indicated that dehydration melting occured at 1250 K. The activation enthalpies before and after dehydration melting are 0.66 eV and 1.56 eV, respectively. When we cooled the sample after dehydration melting to temperatures lower than 1250 K, the activation enthalpy decreased to 0.55 eV. Post-experimental EPMA analysis showed that the melt is adakitic and hydrous. Except for adakitic melt, the other reaction products include garnet and pyroxene.

Dehydration melting of amplibole bearing sample can explain the high conductivity anomaly of 0.1 S/m at temperatures higher than 1250 K. However, the explanation of 1 S/m requires temperatures higher than 1350 K. Our results suggest that the dehydration melting of meta-mafic rocks to explain the high conductivity anomalies of 1 S/m requires high crustal temperature.

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Olivine garnetization - The key to ultrabasic-basic evolution of upper-mantle magmatism: Evidence from melting relations of olivine-clinopyroxene-jadeite system at 6 GPa

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Probability of the upper-mantle ultrabasic-basic magmatic evolution is marked by petrochemical trends with smooth clinopyroxenes and garnets conversions from olivine-normative peridotite to silica-normative eclogite compositions (MacGregor, Carter, 1970). Experimental melting relations of the ultrabasic olivine-orthopyroxene-clinopyroxene-garnet system demonstrate invariant peritectic reaction of orthopyroxene with melt and transition to univariant curve olivine+clinopyroxene+garnet+ melt (Litvin et al., 2016). Experimental melting relations in the join forsterite - jadeite over 4.5 GPa have revealed formation of pyropic garnet (Gasparik, Litvin, 1997). This is promising for deliverance of the Ol+Cpx+Grt+L univariant association from olivine components and transfer from ultrabasic to basic compositions. Experimental study of melting relations of the multicomponent olivine – clinopyroxene – jadeite system using the polythermal sections Ol – Cpx (= Di35Jd75) and Ol80Jd20 – Di65Jd35 at 6 GPa has discovered invariant peritectic reaction of olivine with jadeite components and transition to univariant curve (clinopyroxene ↔ omphacite) + garnet + melt. The peritectic reaction represent the key to ultrabasic-basic evolution of the upper-mantle magmatism and applicable also to evolution of diamond-parental melts-solutions. Finally, the generalized diagram of melting relations for the multicomponent system olivine – diopside – jadeite – garnet is constructed which demonstrates the physicochemical mechanisms providing a control over regularities of fractional ultrabasic-to-basic upper-mantle magmatism and formation of indivisible olivine-saturated peridotite-pyroxenite and silica-saturated rock series. Gasparik T., Litvin Yu.A. (1997). European Journal of Mineralogy, 9, 311- 326. Litvin Yu.A. (2017). Genesis of Diamonds and Associated Phases. Springer, 137 p. Litvin Yu.A., Spivak A.V., Kuzyura A.V. (2016). Fundamentals of the mantle-carbonatite concept of diamond genesis. Geochemistry International, 54, 839-857. MacGregor I.D., Carter J.L. (1970). The chemistry of clinopyroxenes and garnets of eclogite and eridotite xenoliths from Roberts Victor Mine, South Africa. Physics of Earth and Planetary Interiors, 3, 391-397.

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[*] Speaker

Sound velocity measurements in the liquid Fe-S system up to 20 GPa using ultrasonic pulse-echo method

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To understand the structure and composition of the molten core of the terrestrial planets such as Mars, it is important to know the physical properties of liquid Fe alloys at high pressure and high temperature. Sound velocity is a key physical property because it can be directory compared with seismic observations. However, longitudinal sound velocity (Vp) measurements of liquid Fe alloy by ultrasonic methods combined with multi anvil apparatus have been limited to below 8 GPa. Here, we report the latest results of sound velocity measurements in the liquid Fe-S system up to 20 GPa corresponding to the core mantle boundary of the Mars.

High-pressure and high-temperature experiments were conducted at BL04B1 of SPring-8 and NE7A of PF-AR using Kawai-type multi anvil apparatus with a 10/5 cell assembly. We used ultrasonic pulse-echo overlap method to measure sound velocity. The sample lengths were determined by X-ray radiography. Chemical analyses of the recovered samples were conducted using an FE-EPMA-WDS.

The present Vp in the liquid Fe-S system were consistent with those determined by our previous study up to 7 GPa (Nishida et al. 2016). The Vp of liquid Fe-43 at.% S were lower than that of liquid Fe-20 at.% S in all of the conditions of up to 20 GPa. The temperature dependence of Vp was negligibly small, similar to that at low pressures (Nishida et al. 2013; Jing et al. 2014). The experimental P-Vp-T data were well fitted simultaneously to third order Birch-Murnaghan thermal equation of state (Anderson et al. 1989) with large $\mathrm{d}K/\mathrm{d}P$. These results suggest that dissolved S decreases the Vp of liquid Fe under martian core conditions.

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Structure measurement of basaltic glass using neutron diffraction

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Pressure-induced structural evolutions of magmas play a central role in controlling magma mobility in the interior of the Earth. X-ray diffraction technique is a powerful tool for investigating bond lengths and angles of the melt network, and many experiments have been conducted. In order to obtain the detailed structural information, structure factor, *S(Q)*, with a wide Q range is needed. Here, we used a neutron diffraction method for better understanding of the glass structure. The experiments have been conducted using a time-of-flight neutron diffraction at PLANET beamline in Japan Photon Accelerator Research Complex (J-PARC). The staring material is synthesized basaltic glass, and it was compressed using Paris-Edinburgh press up to 8 GPa. The significant oscillation in *S(Q)* was found up to at least 23 Å-1. This means that the resolution in the pair distribution function is Δr=0.27 Å.

With increasing pressure, the basaltic glass displays large shift in the first sharp diffraction peak (FSDP) in *S(Q)* to higher-Q, indicating rapid shrinkage in the intermediate-range ordered structure. In addition, the weakening and broadening of FSDP with pressure was observed. This means the collapse of the intermediate range ordering and may relate to an increase in coordination number of network-forming cation. On the other hand, second sharp diffraction peak (SSDP) showed an opposite behaviour: a significant increase in the intensity of SSDP. This indicates that the magma structure changed to densely packed structure. Corresponding behavior is also found in the pair distribution function, *g(r)*, which is obtained by Fourier transformation of *S(Q)*. I will show a detailed discussion about the pressure dependence of short- and intermediate-range ordered structure of basaltic glass.

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*Speaker

Light-element dependences on structure of liquid Fe at high pressure

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The Earth's core consists of a roughly 96% liquid outer core and 4% solid inner core by volume. Presence of liquid core has been identified not only in the Earth but also in other planets such as Mercury, Mars, and the Moon. The planetary liquid core is considered to be composed of metallic iron with some light elements such as sulfur, silicon, and carbon. Therefore, knowledge on the liquid iron-light element alloys at high pressures is the most fundamental to understand dynamic processes of the core such as core formation and dynamo process which closely relate with nature of liquid iron alloys. In this work, we investigated structure of liquid Fe-Si, Fe-C, and Fe-S alloys at high pressure to understand influence of the light elements on structure of liquid Fe.

We measured structures of liquids Fe, Fe-18.1at.% Si, Fe-28.9at.% Si, Fe-50at.% Si, Fe-14.4at.% C, Fe-25at.% C, Fe-16.2at% S, Fe-23.5at.% S, and Fe-30.3at.% S at the pressures of 3-5 GPa using multi-angle energy-dispersive X-ray diffraction (EDXD) technique with a Paris-Edinburg type large volume press at the beamline 16-BM-B at the Advanced Photon Source.

Structures of liquid Fe-C alloys are basically similar to that of liquid Fe. Liquid Fe-16.2 at.% S also exhibits basic structure similar to liquid Fe, while, at higher S contents, the local structure changes to poorly ordered structure, similarly to those obtained in previous studies. Structures of liquid Fe-Si alloys show mixing behavior between the end member liquids Fe and FeSi. The dissolution of C expands the nearest neighbor distance, indicating that the incorporation mechanism of C into liquid Fe is interstitial type. Similarly, incorporation of small amount of S expands the nearest neighbor distance, while, at high S content, the nearest neighbor distance significantly decreases with increasing S content. In contrast, incorporation of Si shortens the nearest neighbor distance. Our results indicate different nature of incorporation of S, C, and Si in liquid Fe at 3-5 GPa, which may be a key to understand physical properties of liquid iron-light element alloys.

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*Speaker

Thermochemical solution properties of silicate liquids at extreme conditions and implications for the magma ocean.

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All planetary bodies are evolved from a history of accretionary impacts, delivering mass and energy to an otherwise geologically closed system. These impacts generate melting proportional to impactor size. In the case of our moon formation, despite uncertainties regarding the nature of impact and subsequent satellite formation, widespread melting would have been unavoidable. Gaining a better understanding of the properties of a molten mantle system may allow us to contemporarily identify remnants of the magma ocean, in addition to learning how the present-day system evolved. However, the process by which the magma ocean crystallized is still uncertain, including the temperature of liquidus and solidus, crystallization sequence, and compositions of crystallizing phases. Here we take a novel approach towards constraining multi-component freezing equilibria via first principles moleculcar dynamics simulations. Our initial focus has been on computation of the entropy of silicate liquids. The entropy is inaccessible to standard molecular dynamics methods and is therefore a crucial missing ingredient in the first principles computation of phase equilibria. We have investigated methods of computing the two-body configurational entropy deficit, initially focusing on the MgSiO3-CaSiO3 join. We show results for the absolute entropy and the entropy of mixing across the mantle pressure-temperature regime.

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*Speaker

Posters: Earth and Planetary Cores

Sound velocities and density measurements of solid hcp-Fe and hcp-Fe-Si(9wt.%) alloy at high pressure: Constraints on the Si abundance in the Earth's inner core

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The presence of light elements alloyed to iron in the Earth's core is well established, and core formation models based on metal-silicate equilibration point at silicon as one of the major light element in the inner core. However, attempts to constrain Si abundance on the basis of comparison of measured velocities in pure Fe and Fe-Si alloys at high pressure with seismic observations do not provide a unique answer. Available data obtained in the 40-100 GPa range are indeed limited in number and in open disagreement. We carried out sound velocity and density measurements on pure hcp-Fe and an hcp-Fe-alloy with 9 wt.% Si at 300 K up to _˜170 and _˜ 140 GPa, respectively, by inelastic x-ray scattering and x-ray diffraction. The results, combined with previous experiments and calculations, allow a precise determination of the Vp-ρ and Vs-ρ relations for pure Fe and the Fe-Si alloy. The established relations are used to address the effect of Si on the velocities in the Fe-FeSi system in the range of Si concentrations 0 to 9wt.% applicable the Earth's core. Assuming an ideal linear mixing model, velocities vary with respect to those of pure Fe by _˜ +80 m/s for Vp and _˜ -80 m/s for Vs for each wt.% of Si at the inner core density of 13000 kg/m3. The possible presence of Si in the inner core and the quantification of its amount strongly depend on anharmonic effects at high temperature and on actual core temperature.

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Hydrogen and Helium during Earth's core formation

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The accretion of the Earth from primordial material and its subsequent segregation into a planet with core and mantle are fundamental problems in terrestrial and solar system. Many of the questions about the process are still open and much debated. For example, could the core be a reservoir for hydrogen, helium or other noble (rare) gases?
We have developed experimental techniques to simulate the conditions of the formation of the early Earth in a laser-heated diamond-anvil cell (LHDAC). We have studied Ne, He and Ar solubility and partitioning between metal and silicate liquids at high-pressure and temperature up to 20 GPa and 3000 K. Microanalysis of LHDAC samples with Ultra Violet Laser Ablation Mass Spectrometry (UVLAMP) provided for the first time a spatially-resolved depth profile in samples.

Our experimental results show that Ar and He solubility in silicate melts drops at high pressures [1,2]. More importantly, the discontinuous decrease of He solubility in CI-chondrite occurs at a pressure similar to that found for Ar suggesting that the dissolution of noble gases may not in fact be simply a function of effective size, and it is more likely that a single structural change in the host silicate liquid is the dominant factor in determining the solubility.

The experimental results show that helium would have partitioned early into the core during its formation and in proportion to their early abundance, creating a potential reservoir for 3He and 4He. Core He could clearly contribute to the mantle 3He-4He budget – highlighting the exchange mechanisms at the core-mantle boundary through the 4.5 billion years of Earth's history.

In contrast, our experiments show that there is no evidence of important hydrogen incorporation into planetary cores, thus making unlikely for hydrogen to be a major light element of the Earth's core as previously assumed [3].

We will present and discuss our results on metal-silicate partitioning of He and H between chondrite model composition and iron-rich metal liquids up to 20 GPa and the implications that can have on Earth's global geodynamics.

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*Speaker

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Pressure-volume-temperature behaviors for hydrogen content and volume in iron hydride at high pressure and high temperature

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The Earth's core has supposed to be constituted by iron-nickel alloy with some light elements. Hydrogen is one of the most probable candidate among the light elements constituting the Earth's core. Although several studies for iron hydride (FeHx) have been conducted by various methods, precise measurement of hydrogen content in FeHx under high pressure and high temperature conditions has not been conducted due to the difficulty of the experiment. The light elements such as hydrogen cannot be directly observed by traditional methods such as x-ray diffraction method. On the other hand, in neutron diffraction experiments, hydrogen has been substituted to deuterium to avoid strong incoherent scattering. Therefore, the volume and the content of the hydrogen in FeHx are discussed by assumptions through the studies of iron deuteride and several other metallic hydrides. However, such assumptions without precise measurement cause uncertainty. In this study, we conducted high temperature, high pressure neutron diffraction experiment to quantify the hydrogen content and volume in FeHx at J-PARC high pressure beamline (BL11-PLANET). Experiments were conducted in the temperature range of 300-1200K under nearly isobar condition at _˜4, 6, 8 and 11GPa. Double hexagonal close packed (dhcp-FeHx) phase and face centered cubic (fcc-FeHx) phase of FeHx which are high pressure and high temperature phase of hydrogenation of iron were observed and the structure of FeHx and the content of hydrogen in FeHx were optimized using GSAS software by the Rietveld method. Our results show that the hydrogen content in fcc-FeHx was rapidly increased to x=1 with increasing pressure from 3GPa to 10GPa, and there is a strong relation between the hydrogen content of FeHx and its volume increase. And, dhcp-FeHx phase in $>$ 10GPa contains hydrogen exceeding $x>$ 1 by introducing hydrogen into lattice defect sites as seen in hydrogen storage alloys such as iron-titanium alloys.

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*Speaker

On the interior of carbon-rich exoplanets: new insight from Si – C system at ultra-high pressure

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The variability in the mass/radius ratio of the more than 3200 exoplanets discovered so far, is a direct consequence of the large diversity of their internal composition. Exoplanets with a mass between 1 and 10 times the mass of the Earth are typically referred to as super-Earths, and their mineralogical composition depends on that of the protoplanetary disk. The key variable in determining the chemical makeup of such planets is the C/O ratio. Values of C/O ratio smaller than 0.8 correspond to an interior dominated by silicates (e.g. terrestrial planets), whereas for C/O ratios $>$ 0.8 the interior is enriched in carbon. In these C-rich planets, Si may form carbides instead of silicates (Duffy et al., 2015). The detection of planet 55 Cancri e, with a particularly high C/O ratio, has increased the interest in carbon-rich planets. 55 Cancri e has been modelled as a layered structure of carbon, SiC and iron (Madhusudan et al., 2012). However, the accuracy of such type of models suffers the lack of experimental data on the Si – C system at extreme condition of pressure and temperature. Experimental equations of state, is limited to 80 GPa (Nisr et al., 2017) and little is known about subsolidus relation, with only one theoretical study from Wilson and Militzer (2004) at multi-megabar pressures. Here we present experiments on SiC samples by synchrotron X-ray diffraction, in laser heated diamond anvil cell between 30-200 GPa and 300-3500 K. The results show evidences of coexistence of SiC with Si or C, depending on the starting composition, without the appearance of intermediate compounds. Moreover, between 65 and 80 GPa, SiC undergoes a phase transition from the zinc blend structure (B3), to the rock salt structure (B1). This phase transition, also reported in previous literature work (e.g. Yoshida et al., 1993), corresponds to a change in the atoms coordination, and is accompanied by a 20% volume reduction.
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Pre-melting phenomena in an fcc metal

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The Earth's core is believed to be made of an iron-nickel alloy with a few percent of light elements, but its precise structure and composition still remain unknown. Seismological models in the Earth's inner core do not agree with mineralogical models resulting from *ab initio* calculations which predict shear-wave velocities up to 30% greater than seismically observed values. Recent computer calculations revealed that this difference may be explained by a dramatic, non-linear, softening of the elastic constants of Fe just before melting, interpreted as "pre-melting" effects.

To date, computer simulations are the only result on pre-melting of direct applicability to the Earth's core and it is crucial to investigate such phenomena at inner core conditions. Measuring the pressure dependence of pre-melting effects at such extreme pressures and temperatures to the required precision is, however, exceedingly challenging.

We investigated to what extent pre-melting behaviour occurs in the physical properties of other metals at more experimentally tractable conditions. In particular, we determined the thermal expansion of gold (Au) by X-ray powder diffraction from 40 K up to the melting point (1337 K). Au is an ideal test material as it crystallises in a simple monatomic face-centred cubic structure and has a relatively low melting temperature making it a candidate material to study in the laboratory.

Over the temperature range investigated the behaviour of the material may be adequately described by a Gr´uneisen approximation to the zero-pressure equation of state representing the thermal expansion of the "perfect crystal", combined with the theory of thermodynamics of point defects to include the contributions from lattice defects at high temperature ("real crystal"). Au shows a non-linear increase in thermal expansion prior to melting, which is likely due to the generation of point defects over a large range of temperature, beginning at T/Tm> 0.75, which is very similar to what has been observed in the elastic moduli.

From the present study it appears that pre-melting phenomena in *fcc* metals may be less pronounced than those observed in *hcp* metals, such as Fe, at Earth's inner core conditions.

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Stabilization of body-centred cubic iron under Earth's core conditions

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The Earth's solid core is mostly composed of iron. However, the stable phase of iron under inner-core conditions remains uncertain. The two leading candidates are hexagonal close-packed (hcp) and body-centred cubic (bcc) crystal structures, but the dynamic and thermodynamic stability of bcc iron under inner-core conditions has recently been challenged. We demonstrate the stability of the bcc phase of iron under conditions consistent with the centre of the core using *ab initio* molecular dynamics simulations. We find that the bcc phase is stabilized at high temperatures by a novel diffusion mechanism that arises due to the dynamical instability of the phase at lower temperatures [1]. 1. A. B. Belonoshko, T. Lukinov, J. Fu, J. Zhao, S. Davis, and S. I. Simak, "Stabilization of body-centred cubic iron under inner-core conditions", *Nature Geoscience* **10,** 312 (2017).

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*Speaker

The influence of sulfur on the electrical resistivity of hcp iron: implications for the core conductivity of Mars and Earth

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Paleomagnetism and astrophysical studies disclosed the present or past existence of a magnetic field in telluric planets and satellites in our solar system [*Stevenson*, 2003; *Busse and Simitev*, 2015; *Connerney*, 2015]. The core dynamo process that converts kinetic energy into magnetic energy by dynamic motions in the liquid core is the most plausible mechanism for generating a long-lived magnetic field in the rocky planets and satellites [*Stevenson*, 2003]. In order to understand the mechanism of the Earth's core dynamo action, many efforts have been made to determine the electrical resistivity (the inverse of electrical conductivity) of the Earth's core materials. Still, there is no report of the electrical resistivity of iron-sulfur (Fe-S) alloy at high pressures, despite the fact that S is a major light element(s) candidate in the Earth's core because of its depletion in the crust and mantle relative to elements with similar volatilities [*Rama Murthy and Hall*, 1970; *Poirier*, 1994]. In addition, S may be an important light element in the Martian core [*Wanke and Dreibus*, 1988; *Lodders and Fegley*, 1997], and the influence of S on the conductivity of Fe alloy may have important implications for the ancient dynamo action and thermal evolution of the Martian core. In this study, we measured the electrical resistivity of Fe-Si-S alloy with hexagonal-closed-packed (hcp) structure to 110 GPa in a diamond anvil cell (DAC). The obtained electrical resistivity of the hcp Fe-Si-S was analyzed to reveal the influence of S on the electrical resistivity of Fe alloy in combination with the reported resistivities of Fe and Fe-Si alloy at high pressures [*Gomi et al.*, 2013, 2016]. We determined the impurity resistivity that does not have temperature dependence of S in a hcp Fe matrix at high pressures. We found that the impurity resistivity of S is lower than that of Si and unpredictable from the Norbury-Linde rule. Therefore, S is a weaker influence on the conductivity of Fe alloy, even if S is a major light element in the planetary cores. To the best of our knowledge, this is the first demonstration of the electrical and thermal conductivity profiles of the Mars's and Earth's cores including S as a major light element, which would help to study thermal evolution and dynamics in the core of telluric planets.

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Electrical resistivity of liquid iron with high concentration of light element impurities

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The Earth's outer core mainly consists of liquid iron, enriched with several weight percent of lighter elements, such as silicon, oxygen, sulfur or carbon. Electrical resistivities of alloys of this type determine the stability of the geodynamo. Both computational and experimental results show that resistivites of Fe-based alloys deviate significantly from values of pure Fe. Using optical conductivity values computed with the Kubo-Greenwood formalism for DFT-based molecular dynamics results, we analyze the high-P and T behavior of resitivities for Fe-alloys containing various concentrations of sulfur, oxygen and silicon. As the electron mean free path length in amorphous and liquid material becomes comparable to interatomic distances at high P and T, electron scattering is expected to be dominated by the short-range order, rather than T-dependent vibrational contributions, and we describe such correlations in our results. In analogy to macroscopic porous media, we further show that resistivity of a liquid metal-nonmetal alloy is determined to first order by the resistivity of the metallic matrix and the volume fraction of non-metallic impurities.

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*Speaker

Measurements of sound velocity in iron-nickel alloys by femtosecond laser pulses in a diamond anvil cell

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The precise chemical composition of the Earth's core constituting the deepest part of the Earth has been unknown, although it is indispensable for the discussion of the Earth's primordial materials and the formation process. Iron-nickel (Fe-Ni) alloy is believed to be a major component of the core based on the cosmochemical models and the studies of iron meteorites. By comparing the seismic wave velocity profile in the Earth with laboratory data of the sound velocity in deep Earth materials, we are able to decipher the chemical composition and comprising minerals there. Therefore, measurement of sound velocity at high pressures is essential for Earth sciences. In previous studies, sound velocity of pure Fe has been extensively measured from various techniques, while experimental study on sound velocity of Fe-Ni alloy has not been performed in a wide range of Ni content. Here we measured longitudinal wave velocities (VP) of Fe-5wt.% Ni, Fe-15wt.% Ni combining femtosecond laser pulses and a diamond anvil cell, showing that the effect of Ni on the sound velocity of an Fe-based alloy is weaker than that determined by previous experimental study. In addition, our results indicate that light element(s) that induce _˜4.7% and _˜5.2% density deficit and _˜5.5% and _˜4.6% reduction in VP for Fe-5 and 15 wt.% Ni, respectively are required to match the PREM.

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Face-centred cubic iron: ab initio calculations of sound velocities in the lunar core

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Studies, such as the reanalysis of the Apollo lunar seismograms [1], have shown that the Moon has undergone differentiation and possesses a small core. The composition of the lunar core is not well constrained, and many compositional models have been suggested including combinations of iron, nickel, and light elements such as sulphur and carbon [e.g. 1, 2, 3, 4], and other more exotic compositions [5]. Additional constraints are crucial to our understanding of the Moon, including its formation, the dynamics of its interior, and a lunar dynamo.

We use *ab initio* molecular dynamics simulations to calculate elastic constants of face-centred cubic (fcc) iron and iron alloys and hence sound velocities at lunar core conditions, at -˜5-6 GPa and -˜1,300-1,900 K [3]. The results from these simulations will then be compared with the data from the Apollo seismograms and experimental data to help form a description of the lunar interior.

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Laser shock compression of iron and iron alloys studies for planetary science

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An accurate knowledge of the properties of iron and iron alloys at high pressures and temperatures is crucial for geophysics and planetary science. In particular, detailed information on melting curves and solid phases are required to anchor the Earth's thermal profile at the Inner Core Boundary (ICB) and to assess the solid or liquid nature of exoplanets cores. In that context, XFEL sources coupled with high-energy lasers are affording unique opportunities to measure microscopic structural properties at extreme condtions. Here we present recent studies devoted to investigate the solid-solid and solid-liquid transition in laser-shocked iron and iron alloys using both X-ray diffraction and X-ray Absorption Near-Edge Spectroscopy (XANES). Experiment were performed at the MEC end-station of the LCLS facility at SLAC (USA) as well as the EH5 end station of SACLA – Spring-8 facility (Japan).

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*Speaker

Posters: Earth and Planetary Mantles

Lattice thermal conductivity of (Mg,Fe)O solid solutions

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The Earth is cooling since it was born about 4.6 billion years ago. To decipher the thermal history of the Earth, thermophysical properties of the lower mantle materials that constitute more than half the volume of the Earth is of great importance. A number of research suggests that the MgO–FeO solid solution with various chemical composition exists in the lower mantle as consequenses of iron pertitioning among major lower mantle minerals, crystallization of the basal magma ocean, and so on. Iron-rich (Mg,Fe)O magnesiowüstite at the core–mantle boundary may cause regional variation of thermal conductivity of the lowermost mantle due to its distinct iron concentration, which potentially influences the mantle convection style, inner core structure, geomagnetic field reversal frequency and so on. However, there is no systematic study to examine the effect of iron substitution on the thermal conductivity of (Mg,Fe)O solid solution even at ambient conditions. In this study, we measured lattice thermal conductivity of (Mg,Fe)O magnesiowüstite with various iron contents at high pressures, and evaluated its compositional dependence. Our results show much lower lattice conductivity of iron-rich magnesiowüstite than that of MgO and FeO endmembers due to strong iron impurity–phonon scattering. Our data are well reproduced by a model which express impurity-phonon scatterinng effect on the lattice conductivity in a soid solution. Our results will help to estimate the thermal conductivity of (Mg,Fe)O with various composition in the Earth's lower mantle.

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*Speaker

Importance of various type of Al substitutions into bridgmanites under high pressure

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Bridgmanite (Mg-silicate perovskite) (hereafter "Brg") is the most abundant mineral in the lower mantle. The Brg occupies about 70% in the lower mantle (Irifune, 1994), if we assume pyrolite mantle. Because the Al is mainly incorporated into Brg in the lower mantle, the investigation of the Al substitutution mechanism into Brg is very important.
The phase diagram in the system MgSiO3-Al2O3 has been investigated so far based on high pressure experiments (e.g. Irifune et al., 1996; Kubo and Akaogi, 2000).The Al substituion is considered to be Tschermak substitution (Mg2+ + Si4+ = 2Al3+). However the compositions of the synthesized Brg show the deviation from the ideal join of MgSiO3-Al2O3. Some researchers insist that oxygen-vacancy substitution (Si4+ = Al3+ + 1/2Vo, here Vo shows oxygen vacancy.) exist for the Al substitutution into Brg (e.g. Kojitani et al. 2007). In addituion, we recently recognized that Al-bearing Brg can contain significant amount of water up to _~0.8 wt% because of the Al-H coupling substitution (Si4+ = Al3+ + H+). Thus, the Al substitution mechanism into Brg is very complicated.

To clarify the preferred Al substitution mechanism into Brg, we conducted the series of high pressure experiments. The targets to be clarified are as follows: 1) Are there any compositional dependence for the preferred substitutions as a function of Al? That is, which substitution is preferred in low Al or high Al content? 2) If hydrogen exists in the lower mantle, hydrous Brg is preferred to be formed? 3) If there are no hydrogen in lower mantle, which substitution is preferred, Tschermak substitution or oxygen-vacancy substitution? 4) Are there any compositional dependence to be preferred Al substitution in the terms of MgO excess or SiO2 excess condition? 5) What is the reason for the deviation from the ideal join of MgSiO3-Al2O3 in the previous works? 6) What kind of Al-bearing Brg should be existed in the lower mantle?
High pressure and high temprature experiments were conducted at _~28 GPa and _~1600°C using Kawai-type apapratus in GRC, Ehime University. Special care has been done for the sample preparation and capsulation. Especially, to achieve the extremly anhydrous condition in our experiment, the glass rods were used as the starting materials to eliminate the absorbed water on the sample surface. Those results will be presented.

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Electronic configuration and magnetism in FeO at extreme pressure and temperature

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Iron monoxide is a fundamental component in the Earth's interior as the iron endmember of ferropericlase (Mg,Fe)O – the second most abundant mineral in the lower mantle. Moreover, iron monoxide is likely to be the final constituent of the evolution of subducted banded iron formations and might be a source of the low-velocity zones at the Earth's core-mantle boundary (Dobson and Brodholt, 2005). The stability and high-pressure properties of FeO could, thus, determine the fate of banded iron formations and their potential role in processes in Earth and planetary interiors, including controls on redox cycles.

At ambient conditions, FeO crystallizes in the B1 structure and undergoes a phase transition into rhombohedrally distorted B1 (rB1) above 16 GPa (Yagi et al., 1985). The transition is accompanied by the appearance of antiferromagnetic ordering. Although numerous studies were focused on investigation of the electronic and magnetic properties of FeO at high pressures and moderate temperatures, information on the properties at relevant high temperatures is very limited. For instance, the pressure dependence of the Néel temperature – one of the fundamental characteristics of antiferromagnetic materials – was determined only up to 40 GPa under non-hydrostatic conditions (Kantor et al., 2007).

We will present our investigation on the pressure dependence of the electronic and magnetic properties of iron monoxide by means of Synchrotron Ḿ'ossbauer Source spectroscopy in resistively- and laser-heated diamond anvil cells. We employed Single-Crystal X-ray diffraction in order to identify further distortions of the FeO structure at higher pressures. We will discuss the influence of the distortions on the electronic and magnetic properties of FeO and their potential role in the mineralogy, chemistry, and physics of the Earth's deep interior.

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Water and lower mantle phase transformations

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The presence of water in many upper mantle minerals has been shown to have a large effect on their rheology in what is generally known as "hydrolytic weakening". A growing number of studies are finding that incorporating a water dependent rheology into global mantle convection models has a strong effect on global dynamics. However, while there is an abundance of experimental evidence showing that upper mantle minerals deformed under hydrous conditions are significantly weaker than when dry, there is no such experimental evidence for lower mantle minerals.

In this study we use DFT methods to calculate the partitioning of water between different sites in lower mantle minerals (bridgmanite, cubic and tetragonal calcium perovskite, ferropericlase and phase H) which allows us to speculate on the effects of water on lower mantle rheology.

We find that at typical lower mantle conditions water partitions preferentially into bridgmanite but with a mechanism that does not increase the vacancy concentration of bridgmanite and thus is unlikely to affect its rheology.

In cooler conditions, such as in a descending slab, water most prominently partitions into calcium perovskite. The presence of water in calcium perovskite has large effects on the preferred phase and can induce multiple phase transitions at varying depths of the lower mantle depending upon both water content and slab temperature. These transitions are likely to be seismically anomalous and could cause large seismic heterogeneity in descending slabs.
In conditions with large amounts of water (> 5000 ppm) water rich H phases can be formed but these are typically not favoured by the amount of water expected in the lower mantle.

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*Speaker

The stability of anhydrous phase B, Mg14Si5O24, at mantle transition zone conditions

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The stability of anhydrous phase B, Mg14Si5O24, has been determined in the pressure range of 14-21 GPa and in the temperature range of 1100-1700 ◦C with both normal and reversal experiments at high pressures and high temperatures. Our results demonstrate that anhydrous phase B is stable at P-T conditions corresponding to the shallow depth region of the mantle's transition zone and it decomposes into periclase and wadsleyite at greater depth. The decomposition boundary of anhydrous phase B into wadsleyite and periclase has a positive phase transition slope and can be expressed by the following equation, P(GPa)= 7.5 + 6.6 × 10-3T(◦C). This result is consistent with a recent result on the decomposition boundary of anhydrous phase B (Kojitani et al., 2017). However, our phase boundary deviates significantly from theirs at temperatures $<$ 1400 ◦C. Considering the spatial and temporal heterogeneity of mantle compositions, several mechanisms are proposed to produce MgO-rich conditions for the formation of anhydrous phase B in the deep mantle. Upon the cooling of a magma ocean likely formed during the early history of the Earth, a distinctive anhydrous phase B enriched layer might have formed through crystallization and accumulation in the upper part of the mantle transition zone. Subducting carbonate can be reduced in the metal-saturated mantle at depth $>$ 250 km and abundant (Mg, Fe)O oxides should be introduced into the surrounding mantle. Hydrous melting of peridotite may also produce MgO-enriched components. In addition, dissociation of chromite in natural high-P chromitite is likely to produced lots of oxides. We propose that directly touching ferropericlase-olivine inclusions found in natural diamonds might be the retrogressive products of anhydrous phase B decomposing via the reaction Anh-B = Olivine + Periclase. This decomposition may occur during the transportation of the host diamonds from their formation depths of $<$ 500 km in the upper part of the mantle transition zone to the surface.

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Posters: Experimental and Analytical Techniques

Development of rotational diamond anvil cell for deformation experiments under high pressure conditions corresponding to the lowermost mantle

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A pressure range enabled to perform the deformation experiments has been limited due to a technical reason. Extending the pressure range is necessary to understand the dynamics and evolution of Earth's deep interior. A rotational diamond anvil cell (rDAC) is the most suitable deformation apparatus to investigate the rheological properties of deep-Earth materials such as conditions corresponding to the lower mantle and core. The upper anvil of the rDAC rotates relative to the lower anvil and gives the torsional deformation to a sample (Nomura, Azuma et al., 2017). Therefore, the rDAC can theoretically produces an infinite strain to the sample. We report the development of the rDAC and its availability as a deformation apparatus.

In this study, we attempted to improve the pressure range and the prevention of a slip between the sample and the anvil in the deformation experiments using the rDAC. The starting material was a mixture of bridgmanite and ferropericlase. This starting material was grooved by FIB and a platinum strain marker was embedded into each sample. The experimental conditions were P = 35–137 GPa, room temperature and strain-rate of 5.6×10ˆ-5–1.7×10ˆ-4 sˆ-1. Four types of the diamond anvil designs were tested to evaluate the performance with respect to slip between the sample and the diamond anvils. These deformation experiments were conducted in Japan Synchrotron Radiation Research Institute (SPring-8) and 3D visualization of the strain-marker in the samples were performed using X-ray laminography (Nomura and Uesugi, 2016).

The geometry of strain-marker in the deformed samples showed a nearly simple shear deformation, indicating that this apparatus can deform the sample with large strain under high pressure conditions, corresponding to those of core-mantle boundary (CMB). The rotation angle of the strain-marker in the deformed samples was compared to the rotation angle of the upper anvil. This comparison indicated that the one of the optimizing anvil (the diamond anvils with deep grooves) can prevent the slip between the upper anvil and samples.

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Target fabrication using films depositions for high-pressure planetology studies

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The ERC Planet Dive aims at providing experimental references for phase diagrams, equations of state and melting properties of planetary materials up to the TeraPascal pressure range (1 TPa = 1012 Pa = 10 Mbar). Two mains issues have been identified in order to complete successfully this task:
-A large range of sample with various chemical compositions (Fe, Si, Mg, Ca elements carbide and oxide alloys) and crystalline state is necessary for the planetary materials study.

-The multilayer targets fabrication needs to be perfectly control in order to monitor the compression evolution into the sample at such pressure and to obtain results repeatability.

To answer to this challenge, IMPMC has made the choice to develop thin films deposition and characterisation. Magnetron sputtering process allows reaching good stoichiometric control of the alloys deposits. Moreover, O2 or N2 partial pressure could be added to the argon gasflow reacting in the plasma to obtain oxydes or nitrides of metallic sample. Fe, FeOx (figure 1), FeSixCy, and MgFexOy depositions has been achieved with the reactive sputtering.

Another process used, the electron beam PVD (Physical Vapor Deposition) allows us the deposition of oxydes (AlOx, CaTiO3) and salts (LiF, KCL) from solid precursors. Thin metal or Parylen (with another process) layers could also be deposit on the multilayer assembly as an ablator.

Ion polishing or FIB (Focused Ion Beam - figure 1) are used to obtain high-quality cross-section for the SEM or TEM observations. A confocal/interferometer microscope allows us to obtain 3D image and surface rugosity of the sample. Easy thickness monitoring of the sample can also be reached with this technique.

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*Speaker

Community Extreme Tonnage User Service (CETUS): A 5000 ton press open research facility in the United States

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Large sample volume 5000 ton multi-anvil presses have contributed to the exploration of deep Earth and planetary interiors, synthesis of ultra-hard and other novel materials, and serve as a sample complement to pressure and temperature regimes already attainable by diamond anvil cell experiments. However, no such facility exists in the Western Hemisphere. We are establishing an open user facility for the entire research community, with the unique capability of a 5000 ton multi-anvil and deformation press, HERA (High pressure Experimental Research Apparatus), supported by a host of extant co-located experimental and analytical laboratories and research staff.

We offer wide range of complementary and/or preparatory experimental options. Any required synthesis of materials or follow up experiments can be carried out controlled atmosphere furnaces, piston cylinders, multi-anvil, or experimental impact apparatus. Additionally, our division houses two machine shops that would facilitate any modification or custom work necessary for development of CETUS, one for general fabrication and one located specifically within our experimental facilities. We also have a general sample preparation laboratory, specifically for experimental samples, that allows users to quickly and easily prepare samples for ebeam analyses and more.

Our focus as contract staff is on serving the scientific needs of our users and collaborators. We are seeking community expert input on multiple aspects of this facility, such as experimental assembly design, module modifications, immediate projects, and future innovation initiatives. We've built a cooperative network of 12 (and growing) collaborating institutions, including the Consortium for Materials Properties Research in the Earth Sciences (COMPRES).

CETUS is a coordinated effort leveraging HERA with our extant experimental, analytical, and planetary process modelling instrumentation and expertise in order to create a comprehensive model of the origin and evolution of our solar system and beyond.

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Development of the falling-sphere technique for measuring the viscosity of liquid iron-sulfur alloys at high pressures

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Sulfur is one of the important potential terrestrial planetary core materials and knowledge of the viscosity of liquid iron-sulfur alloys at high pressure is important for understanding the properties such as the convection and geomagnetic evolution of the Earth's outer core. Measurements of the viscosity of liquid iron-sulfur alloys have been attempted using the X-ray radiography falling-sphere method, which measures the terminal velocity of a marker sphere sinking in the liquid sample. However, in the viscosity measurement of liquid iron-sulfur alloys, a chemical reaction between the metal marker sphere and the liquid is a serious problem. In this study, we have developed a newly alumina coated metal marker sphere (Pt), whose diameter is 100 μm with a very thin alumina layer (2 μm in a thickness). Use of the alumina coated sphere can prevent such a chemical reaction and the viscosity of liquid iron-sulfur alloys can be successfully obtained at higher pressures. Also in order to reliably estimate the viscosity of the Earth's outer core, the precise activation energy and activation volume are required over as wide a range of pressure as possible. We have developed a diamond/SiC composite anvil for the multi-anvil press, which has good X-ray transparency and has superior hardness compare to a conventional tungsten carbide (WC) anvil. Combining the diamond/SiC composite anvil with the X-ray radiography falling-sphere method, the marker sphere sinking in the liquid can be observed through the diamond/SiC composite anvil. Therefore, since the effective view range required for the X-ray radiography falling-sphere method is not limited by narrowing the anvil gap of the multi-anvil press, the pressure range of the viscosity measurement can be expanded. Here we present the development of the falling-sphere technique and the results of the viscosities of liquid iron-sulfur alloys at pressures up to 14 GPa.

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X-ray focusing optics development toward sub-micro x-ray diffraction

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The combination of advanced synchrotron x-ray techniques and high-pressure methods provide new level of high pressure studies including mineral physics, condensed matter physics, and high-pressure chemistry. The beamline BL10XU at SPring-8, Japan, has been dedicated to high-pressure powder x-ray diffraction in a diamond anvil cell (DAC). As the accesible pressure and temperature range expands, characterization of minute samples with micron-size requires well-focused and intense synchrotron x-ray probe. We have intensively developed the x-ray optics on focusing for the past decade.

In BL10XU, x-ray beam is focused down to micro-size (2-3 μm) by the x-ray focusing optics of compound refractive lenses. The pressure-temperature (PT) range accessible in the DAC exceeds high-P/high-T conditions 300 GPa and 5,000 K and high-P/low-T conditions above 200 GPa and below 10 K, respectively, and micro x-ray diffraction experiments are performed under such as the extreme conditions. For instance, the structure and electrical resistivity of iron was measured under the core conditions (Ohta et al., 2016), and the crystal structure of high-pressure hydrogen sulfide with high superconducting temperature near 200 K was investigated above 150 GPa (Einaga et al., 2016).

More recently, high pressure experiments increase not only with a single stage type DAC but also with a double stage DAC configuration (Sakai et al., 2015), and the use of a nano-probe is required with spatial resolution for x-ray diffraction. Now we have been upgrading the x-ray focusing optics using compound refractive lenses for generating a sub-micro beam. Here we present overview of the current status of instruments and research for x-ray diffraction on BL10XU, and recent development projects will be discussed.

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*Speaker

High pressure neutron diffraction experiments for icy materials with diamond anvil cell

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Neutron diffraction experiments under high pressure have been limited because intensity of neutron scattering is weak and large sample volume is required. Recently, high intensity pulsed neutron beam is produced by the spallation neutron sources such as the MLF, J-PARC in Japan and the SNS, ORNL in USA. Then, new high-pressure neutron-scattering technics using high intensity neutron beam have been developed. For example, new design of diamond anvil cell (DAC) was developed and the neutron diffraction data up to 94 GPa were obtained in the SNAP beamline (BL3) at SNS (Boehler et al., 2013).

At present, we are also developing the DAC for neutron diffraction experiments at the PLANET beamline (BL11) in MLF, J-PARC. The conically shaped diamond anvil with culet of ϕ1.5 mm was applied. The pressure of 29 GPa was generated and we succeeded in obtaining the neutron diffraction data of ice VII. Now we are proceeding with the developing to generate higher pressures. In addition, we have made an attachment to load the gas into the DAC using a gas loading system at NIMS in Japan. We are planning to load hydrogen gas with water into the DAC to perform the high pressure neutron experiments for hydrogen hydrate.

In order to analyze the neutron diffraction data, Guthrie et al. (2017) suggested that the Bragg condition of the diamond must be considered when single crystal diamond is used as the anvil. It is because a part of the incident beam is lost by the Bragg refraction of the diamond anvils before reaching the sample, which modifies the diffraction intensities from samples. We have measured the transmission of the DAC, and corrected the intensity loss by the methodology invented by Guthrie et al. (2017). Subsequently, we will establish the correction method for data taken at PLANET beamline.

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*Speaker

A waveguide-based flexible CO2 laser heating system

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The laser-heated diamond-anvil cell (DAC) allows for simulating the pressure/temperature conditions of the Earth mantle and has been extensively used in conjunction with laboratory probes and synchrotron-based methods to make in-situ measurements of physical properties of mantle materials. Based on recent developments regarding the availability of compact high-power fibre lasers emitting radiation with a wavelength of about 1 μm, compact "portable" laser heating systems have been developed that drastically simplified the application of laser-heating and opened the perspective for new type of experiments. However, many (mantle) minerals only weakly absorb laser radiation with 1 μm wavelength. In addition, inhomogeneous distribution of iron (clustering), that is mostly causing laser absorption, may lead to substantial spatial variations in sample temperature. CO2 laser-heating (10μm wavelength) overcomes most of these problems, but, in absence of available fibre optics, its application has been restricted to (few) stationary heating setups. The recent availability of 10 μm wavelength transmitting waveguides opens the possibility to design flexible CO2 laser heating systems that can be conveniently used in combination with a variety of experimental probes. Here we present results of test experiments, where a fan-cooled CO2 laser was coupled to a commercially available Hollow Silica Core Waveguide. In addition to the transmitted laser radiation, visible laser light is transmitted in the cladding of the fibre and serves as a visible guide beam during laser alignment. We will discuss results of different experiments to heat metals and oxides both in air and in diamond-anvil cells. In the future, we plan to integrate both the visualization and the temperature measurement optics into the cage-based system in order to construct a fully self-standing flexible CO2 heating system, offering unique perspectives for future experimental research using diamond-anvil cells both in laboratory environments and at synchrotron facilities.

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*Speaker

Viscosity measurement with an X-ray radiography falling sphere method using Diamond/SiC composite anvils in the Kawai-type high-pressure apparatus

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Using diamond/SiC composites anvils prepared with hot isostatic pressing, we have been attempting their practical application to high-pressure anvils addressing their transparent properties to X rays. Cubes of the composites with 14 mm edge length were fabricated and used as the second stage anvils in a Kawai-type high-pressure apparatus. Because the diamond/SiC composites are transparent to X rays, the present anvils are applicable not only to energy dispersive diffraction experiments but also to angle dispersive diffraction experiments and radiographic studies that need a larger window for X-ray passes. In the present study, we measured the melting temperatures and the viscosities of KCl and NaCl under high pressure by an X-ray radiography falling sphere method using synchrotron radiation and the diamond/SiC composites anvils,

High-pressure and high-temperature falling sphere viscometry experiments were attempted in the SPEED-MkII system. Because the present diamond/SiC composite is an insulator, we used the hybrid anvil system with four diamond/SiC and four WC 14 mm cube anvils for heating. Electric power is supplied via WC anvils to furnaces in a high-pressure cell. Pressure generation for anvils with a truncation edge length of 3.0 mm was examined. A high-pressure cell assemblage developed for viscosity measurements was used with minor modifications according to the feedback from each run. We used TiB2 and LaCrO3 cylindrical heater. The pressure-transmitting medium was semi-sintered MgO and the gasket material was pyrophillite. KCl and NaCl powder together with Mo and W spheres was charged in an Al2O3 sample capsule. By using the two spheres with different density, we also attempted density measurements of these liquids. We used a newly developed high-speed radiography system that makes it possible to capture images at an interval of about 4 msec/picsel.

The obtained viscosity of liquid KCl as a function of pressure shows non-linear increase around 2 GPa and this may indicate a local structure change corresponding to the B1-B2 transition that occurs in the solid phase at the same pressure range. Due to the mechanical strength of our diamond/SiC composites anvils, the maximum pressure in the present study was limited to about 17 GPa. The viscosity of NaCl shows gradual increase in the present pressure range.

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*Speaker

Yield strength of rocksalt structures at high-pressure using Raman piezometry

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Measuring yield strengths of condensed materials under non-hydrostatic compression provides essential constrains on their behavior under extreme mechanical efforts ranging from those encountered in planetary interiors to those in boundary lubrication. Raman frequencies of quartz are used to evaluate deviatoric stresses in rocksalt-structure media in diamond-anvil cell experiments to pressures up to 20 GPa. The piezospectroscopic effect in quartz is modeled by first-principles calculations. Non-hydrostatic stresses measured in halogen salts give yield strength estimates in the B1 (NaCl), and B2 structure (KCl and KBr). Raman measurements in MgO show that yield strength is consistent with former radial X-ray diffraction measurements. Radial pressure and deviatoric stress distribution in the DAC is mapped and used to discuss applicability of former determinations of yield strength.

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Dynamic compression experiments with the new High Energy Density Science (HED) instrument at the European XFEL

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With the use of the new experimental facility, the High-Energy Density Science (HED) instrument at the European XFEL it will be possible to investigate matter at extreme conditions like those found inside of exoplanets (Appel et al., 2014; Tschentscher et al., 2017). We will be able to study the model system MgO at pressures of up to 1 TPa and several 1000 K through the temporal pulse shaping capability of the optical laser DIPOLE100X, which will allow quasi-isentropic compression of material, reaching off-Hugoniot high pressure states. These states will help us understand the basic compositional and structural properties of large, terrestrial exoplanets, so-called 'Super-Earths'. Sample design will consist of polycrystal MgO to be deposited as successive coatings directly on a pressure window (LiF). Typical thickness of the sample should be varying from a few μm up to a maximum of 20 μm to ensure homogenous pressure distribution. Specific heating procedures during the process of deposition will enhance the XRD signal. Experimental results will be compared to *ab initio* hydrodynamic simulations to benchmark experimental key phases at the relevant conditions (Cebulla and Redmer, 2014). Ultimately, we are going to obtain equation-of-state (EOS) data for MgO including its melting curve. First simulations via the hydrocode *ESTHER* (Colombier et al., 2005) reveal experimental conditions, in which peak pressures of $>$ 6 Mbar and temperatures of more than 10000 K can be achieved for MgO of 5 μm thickness, a 200 μm square pulse, pulse durations of 5 ns, incident beam angle of 20 degrees and consequently laser intensities of over 7e13 W/cm2. The experimental achieved P-T conditions will be equivalent to those in the inner Earth and in larger rocky planets and ultimately help to understand the compositional and structural properties within these objects.

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*Speaker

Germanium coordination and bond distances in compressed amorphous GeO2 up to 100 GPa by valence-to-core X-ray emission spectroscopy

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The application of valence-to-core X-ray emission spectroscopy (vtc-XES) to DAC experiments is a developing field of research. This probe allows insight into the pressure evolution of electron binding energies and electronic transition probabilities.

In the case of germanium oxides, this information can be extracted from the oxygen 2s -> germanium 1s crossover transition emission line, whose energy and intensity are directly proportional to the germanium coordination and the Ge-O bond distances, respectively. This makes vtc-XES a powerful tool for germanium oxides at high pressure, complementary to X-ray diffraction (XRD) and extended X-ray fine structure absorption spectroscopy (EXAFS) measurements. The information from measured and modeled vtc-XES spectra is extracted in a simple straightforward way, without additional parameters or assumptions concerning density.

We compressed amorphous GeO2 up to 100 GPa in diamond anvil cells (DAC) and measured germanium valence-to-core X-ray emission spectra. The 6-fold coordination is reached at 20 GPa. At about 50 GPa, a further coordination increase is observed, and the average coordination reaches about seven at 100 GPa, in agreement with the recent XRD study of Kono et al. 2016.

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Double-Stage Diamond Anvil Cell Technique for Ultra-High Pressure Generation - Possibilities and Difficulties -

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In 2012 Dubrovinsky and his colleagues have reported the generation of 620 GPa (1) using double-stage diamond anvil cell technique (ds-DAC). This technique looks to be a very promising way to generate static high pressures beyond the limit of conventional diamond anvil cell and many other groups have tried to generate high pressures using similar technique (2-4). Unfortunately, however, by now no other groups have succeeded in generating pressures beyond 500 GPa, although the first group has reported the generation of further high pressures up to 1 TPa (5). We have been working to establish a technique to achieve pressures beyond 500 GPa in a reproducible manner by adopting the concept of ds-DAC. Although we made more than 20 runs, none of them has exceeded 500 GPa. In this talk we will report various possibilities and difficulties associated with this ds-DAC technique based on the various observations obtained in our study.

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*Speaker

XRD and XAFS Debye-Waller factors in high-pressure perovskite-type compounds

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The perovskite-type ABO3 compounds are the analogues of lower mantle minerals. Single crystals of perovskite-type compounds, MgSiO3, CaGeO3, PbTiO3 etc, were synthesized in a cubic anvil type apparatus under high pressures and temperatures [1]. High temperature single crystal XRD and XAFS measurements were carried out at temperature up to 900 K, leading to the analysis on dynamic and static parts in Debye-Waller factors. Mean-square displacement (MSD) and mean-square relative displacement (MSRD) can be determined by XRD and XAFS methods, respectively. The MSD and MSRD for the A site atom is uniquely large, which is one reason for the Clapeyron's curve (dT/dP) of phase boundary to perovskite-type structure having a negative slope. The potential coefficient, α in V(u)= αu2/2+βu3/3!, for the A atoms are significantly smaller than those for the framework vibration. The MSRD contains the contribution from the MSD of both X-ray absorbing (a) and backscattering (b) atoms and the displacement correlation function (DCF). The ratios of 2DCF/ (MSDa + MSDb) for Ca-O and Ge-O in CaGeO3 are about 0.57 and 0.77, respectively. These values are normal in comparison with various compounds. Weak contributions of DCF to MSD in Ca-O bond indicate the increase in ionic character in the perovskite-type structure. The estimated values of Debye temperature ΘD for Pb and Ti are 154 and 467 K in tetragonal PbTiO3 phase and decrease 22% for the high temperature phase. The deviation from the linear temperature dependence in Debye-Waller factors in several ferroelectric tetragonal phases can be interpreted as a precursor phenomenon of the corresponding phase transition. Disturbance of Debye-Waller factor for O is observed at the vicinity of transition point. The O site in PbTiO3 and Ti site in BaTiO3 include the clear configurational disorder in the cubic phase [2]. It was observed in several high-temperature perovskite-type phases that the atom for B or O sites occupies on the off-center position in each site. The polar local positional distortions are regarded as the cause of the para-electricity. It could be suggested that statistical distributions of atoms do not occur in A site, but the A atoms have uniquely large thermal vibration amplitudes.

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Measurement of the Temperature Distribution on the Surface of the Laser Heated Specimen in a Diamond Anvil Cell System by the Tandem Imaging Acousto-Optical Filter

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The laser-heated diamond-anvil cell (LH-DAC) is the only experimental tool able to create extreme static pressures ($P > 100$ GPa) and temperatures ($T > 3000$ K) and it has had a major impact in high-pressure research and geophysics.

The conventional way to determine the temperature of a laser-heated specimen is by measuring the radiation emitted from the heated specimen using a diffraction spectrometer. However, those measurements only provide the temperature of the heated spot averaged over its area. This a technique works perfectly only for a uniform temperature distribution. However, the temperature under a laser has significant non-uniformity. Recently, flat top laser heating was used to study the elastic properties of platinum alloy by measuring the velocity of the skimming acoustical wave in iron at at 2580 K and 22 GPa in a DAC. For such measurements it is important to use an area with a flat temperature distribution. Further progress in the development of the laser heating techniques requires knowledge of the 2-D temperature field in a material induced by laser beam radiation.

Conventional techniques for the measurement of 2-D temperature distribution based on calibration of the digital signal from the camera in the infrared or visible ranges are not applicable for DAC due to priori unknown and non-uniform emissivity distribution in the sample. Several techniques were proposed to measure temperature distribution in a specimen heated by a laser . Recently, a multispectral imaging radiometry (MIR) system for measuring temperature gradients of specimens under high pressure heated by laser in a DAC (LH-DAC) was developed by Campbell.We demonstrate that combining the laser heating system in a diamond anvil cell (LH-DAC) with a tandem acousto-optical tunable filter (LH-DAC-TAOTF) allows measurement of the temperature distribution under laser heating of a specimen under high pressure in a DAC. The main component of the system is an imaging TAOTF synchronized with a video camera. The use of the TAOTF also makes it possible to visualize the infrared (1064 nm) laser beam,

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[*] Speaker

which is invisible to the human eye. The distribution of the temperature $T(x,y)$ was then determined on surface of two Pt plates loaded in DAT at high pressures by fitting the actual signal to Planck's equation at each point of the specimen's surface

Posters: Volatiles in Planetary Interiors

Water incorporation in transition zone minerals, wadsleyite and ringwoodite: A study using ERDA (Elastic Recoil Detection Analysis)

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The transition zone is potentially an important water reservoir within the Earth. Indeed, transition zone minerals, namely wadsleyite and ringwoodite, can contain up to 3.2 wt% H2O by weight (Inoue et al., 1995). In recent years, we have been working on extending the capabilities of measurements of water in minerals using other techniques than Fourier Transform Infrared spectroscopy (FTIR) like Raman spectroscopy (Bolfan-Casanova et al., 2014) that allows the use of very small probing beams under reflection geometry, but also ERDA (Elastic Recoil detection Analysis, Bureau et al., 2009; Withers et al., 2012) that allows quantification without the use of any standards. The main problem of using FTIR on wadsleyite and ringwoodite is that these phases are often too absorbing to allow proper quantification of water. Also, whenever working on realistic, i.e. complex, compositions, samples end up having small grain sizes that are difficult to deal with FTIR when the samples are polyphasic. Thanks to ERDA, we calibrate the Raman spectroscopy for quantifying water in wadsleyite and ringwoodite. We will also discuss the incorporation mechanisms of H in both phases.

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[*] Speaker

Fluorine and Chlorine in the transition Zone

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We report concentrations of Fluorine (F) and Chlorine (Cl) in synthetic wadsleyite (Wd) and ringwoodite (Rw). Synthesis were performed under pressures (14–22GPa) and temperatures (1100–1400°C) relevant to the transition zone (TZ: 410–670 km depth) using multi-anvil press experiments in MLV Clermont-Ferrand, France and in BGI Bayreuth, Germany. F, Cl and H contents were measured using Particle Induced Gamma-Ray Emission (PIGE), Particle Induced X-ray Emission (PIXE) and Elastic Recoil Detection Analysis (ERDA) respectively, using a nuclear microprobe at CEA Saclay. Results show that F (up to 850 ppm wt.) and Cl (up to 200 ppm wt.) are concentrated together with H2O in both Wd and Rw (Roberge et al., 2015; 2017). Cl content in Rw and Wd is significantly higher than in other nominally anhydrous minerals of the upper mantle (olivine, pyroxene, garnet), when we found that F is also concentrated in hydrous olivine (up to 1700 ppm wt., Crepisson et al, 2014). With these data we put constraints on the F and Cl budget of the deep Earth, we propose that the TZ may be a major repository for major halogen elements in the mantle. We also show that both F and Cl abundances are underestimated for the bulk silicate Earth (BSE). We propose maximum abundances for the BSE of 59 ppm wt. F and 37 ppm wt. Cl, these abundances are higher than the values proposed by McDonougth and Sun in 1995, of 25 and 17 ppm wt. respectively. New results on F-bearing ringwoodite will be presented at the meeting.

Crepisson et al., 2014. Clumped fluoride-hydroxyl defects in forsterite: implications for the upper-mantle, EPSL 390, 287-295.

McDonough, W.F., Sun, S., 1995. The composition of the Earth. Chem. Geol.120, 223–253.

Roberge et al., 2015. Is the transition zone a deep reservoir for fluorine?, EPSL, 429, 25-32.

Roberge et al., 2017. Chlorine in wadsleyite and ringwoodite: an experimental study, EPSL 467, 99-107.

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High-pressure high-temperature study of solid benzene

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Benzene is one of the basic compounds in organic chemistry, the building unit of aromatic compounds, that are believed to be the most abundant organic molecules in the Universe (Ehrenfreund and Charnley, 2000; Tielens, 2008) possibly due to electron delocalization over their carbon skeleton, which makes them remarkably stable (Ehrenfreund and Charnley, 2000). The formation of aromatic hydrocarbons in space is usually associated with irradiation-driven polymerization of smaller hydrocarbons (Joblin and Tielens, 2011). Large aromatic hydrocarbons have a huge influence on the heating of cosmic gas and the degree of interstellar space ionization (Tielens, 2008). Moreover, aromatic hydrocarbons as well as amines and amino acids were found in meteorites (Becker et al., 1997; Oro et al., 1971). Carbonaceous chondrites containing aromatic hydrocarbons in their matrix could serve as a source of extraterrestrial organic prebiotic material during the period of heavy bombardment of the inner Solar System 3.8–4.5 billion years ago (Anders, 1989; Chyba and Sagan, 1992; Chyba et al., 1990). We have refined crystal structure and defined melting and decomposition parameters of benzene at 1.5–8.2 GPa and 298–923 K using multianvil apparatus and *in situ* neutron and X-ray diffraction. Our data show the minor temperature effect on the compression behavior of deuterated benzene at 7.8–8.2 GPa. At 3.5–4.0 GPa we observed the deviation of D atoms from ring plane with rising temperature caused by the displacement of benzene molecules and decrease of intermolecular van der Waals bond of π-conjuncted carbon skeleton and the deuterium atom of adjacent molecule. Benzene decomposition was defined at 1.5–8.2 GPa between 773–923 K. The benzene decomposition products consist of carbonaceous material. Triple point between solid, fluid and decomposed state of benzene was defined at _˜3.5 GPa and _˜773 K. Phase diagrams of benzene, naphthalene, pyrene and coronene show consistent shift of triple point between fluid, solid and decomposed state to lower pressures. The equalities of carbonization parameters for aromatic compounds at pressures $>$ 4 GPa are related to the identity of molecular packing at these conditions.

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Hydrogen bond symmetrisation in filled ice methane hydrates under high pressures

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We report the results of Raman spectroscopy measurements and molecular dynamics simulation including nuclear quantum effects on methane hydrate high pressure phases up to 150 Gpa. We have found signatures of hydrogen bond symmetrisation and new high pressure phases.

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*Speaker

Hot-pressing and analysis of polycrystalline specimens of hydrated wadsleyite (β-Mg2SiO4) for acoustic velocity measurements.

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The nominally anhydrous mineral (NAMs) phases – olivine (α), wadsleyite (β) and ringwoodite [(γ-Mg,Fe)2SiO4), believed to be stable in the Earth's upper mantle and the transition zone (410-660 km depth), incorporate considerable amounts of water as structurally bonded OH, causing changes in their physical properties, including elastic wave speeds and elastic properties. Experimental and theoretical studies indicate that wadsleyite (β-Mg,Fe)2SiO4) in particular, can accommodate varying amounts of water up to 3.3 wt.%, depending on the pressure (P) and temperature (T) and phase assembly. The elastic properties of hydrated mantle mineral are essential for assessing mantle composition based on matching laboratory velocity and density profiles for mantle phases with data from regional seismic studies, to assess the role of water in the lateral inhomogeneity observed from seismic tomographic studies of the Earth's mantle, and to improve our general understanding of the Earth's mineralogical and chemical composition. The data are also valuable for assessing the Earth's water budget, and for locating the water repositories in the Earth's interior. Due to the significant difficulty in synthesizing large single crystals of the high pressure phases of mantle minerals for ultrasonic studies, we have adapted techniques to fabricate optimum acoustic-quality synthetic polycrystalline specimens of hydrous wadsleyite (β-Mg2SiO4) suitable for ultrasonic studies. Results for polycrystalline specimens of hydrous β-Mg2SiO4 containing 0.5 wt.%, 0.8 wt.% and 1wt.% OH, respectively hot-pressed in a multi-anvil press, and characterized by Fourier transform infrared (FTIR) spectroscopy, Raman Spectroscopy, non-destructive X-ray diffraction, scanning electron microscopy (SEM), immersion bulk density measurements and bench-top acoustic velocity measurements are presented, including results of preliminary high pressure ultrasonic studies carried out on the13-ID-C,D beam line at the Advanced Photon Light Source (APS) in Chicago, in the USA.

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Posters: Phase Relations, Phase Transitions, and Kinetics

Hydrothermal Synthesis of GTS-type Sodium Titanosilicate and its Sm3+ Ion Exchange

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Grace titanosilicates (GTS), represented by pharmacosiderite, have three dimensional tunnel-type structures. Na-GTS ($Na_4Ti_4Si_3O_{16}\cdot 6H_2O$) crystallizes as a rhombohedral phase (space group ; a = 7.812 Å, α = 88.79∘) close to cubic system. In this structure, four TiO_6 octahedra linked by edge-sharing form a Ti_4O_{16} cubic cluster; the clusters are linked through SiO_4 tetrahedra to form a three-dimensional framework with an interconnected pore system of 8-ring channels, occupied by the alkali-metal ions and adsorbed water molecules. The radioactive waste water continues to accumulate at the crippled Fukushima Daiichi Nuclear Power Plant. It is important to investigate the Sm^{3+} ion exchange properties of Na-GTS for the application of GTS to the removal of Sm radioisotopes from the radioactive waste water. In the present study, Sm^{3+}-exchanged form [$Na_{4(1-x)}Sm_{4x/3}(Ti_4Si_3O_{16})\cdot nH_2O$] of Na-GTS prepared hydrothermally are investigated by powder XRD to examine the occupied positions of Sm^{3+}.

The starting materials for the hydrothermal synthesis were NaOH, amorphous SiO_2 fine powder and $TiCl_4$ aqueous solutions. For the synthesis of Na-GTS, the starting mixtures with the molar ratios of TiO_2/SiO_2 = 0.32 and Na_2O/TiO_2 = 5.62 were hydrothermally treated at 100 ∘C (0.23 MPa) according to the reported procedure. The Sm^{3+}-exchanged forms were obtained by shaking of the synthesized Na-GTS (0.5 g) in the aqueous solution of $SmCl_3$ (25 mL) at 25 ∘C for 6 hours. The concentration of Sm^{3+} in the aqueous solution was varied in the range from 0.01 to 0.5 M. The obtained samples were filtrated, washed and dried at 80 ∘C, after which they were examined by powder XRD. The Sm concentrations in the supernatant solutions were analyzed with atomic absorption spectrometry to evaluate the ion-exchange amounts.

The sample with the composition x = 0.95 was obtained after the treatments of Na-GTS in 0.5 M $SmCl_3$ aqueous solutions. The increase in concentration of the $SmCl_3$ aqueous solution increases the exchange amount. The comparison of the observed and simulated XRD patterns suggests that Sm^{3+} ions are almost equally distributed on both 4e and 6g sites in the cavities of GTS framework.

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[*] Speaker

Aragonite-II and CaCO3-VII – new high-pressure phases of CaCO3

Pavel Gavryushkin * [1,2], Naira Martirosyan [3,4], Sergey Rashchenko [3,4], Sergey Lobanov [3,5,6], Konstantin Litasov [3,4], Talgat Inerbaev [7], Zakhar Popov [8], Anna Likhacheva [3]

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Due to principal importance for mantle geology, high-pressure field of CaCO3 phase diagram have been studying since invention of high-pressure technique. However, this investigation is far from been completed. In the present work, we show the results of targeted theoretical and experimental search which reveal two new polymorphs.
Calculations on crystal structure prediction were performed based on evolutionary algorithms (USPEX package) and density functional theory (VASP code) in the pressure range 20-100 GPa, with the most thorough search around aragonite to post-aragonite transformation (30-50 GPa). This calculations reveals the new structure with P21/c symmetry, which is most energetically favourable in the pressure range 32-46 GPa. Analysis of atomic arrangement shows that found P21/c structure is the analogue of deformed aragonite, based on which we called it aragonite-II. This analysis also shows that founded earlier P21/c-l [Pickard and Needs, 2015] structure is similar to CaCO3-VI and can be considered as its superstructure with a = a', b = b', c = 2c'. CaCO3-VI was synthesised experimentally on cold compression of calcite [Merlini et al., 2012], our calculations shows that it is metastable in all pressure-temperature range.

P-T phase diagram calculated based on density of sates of phonons shows, that stability field of aragonite-II decreases with pressure, inclining at triple point aragonite-postaragonite- aragonite-II at 33 GPa and 1200K.
Performed at 13ID-D of GSECARS (Advanced Photon Source) in situ diamond anvil cell experiments confirm theoretical phase diagram and reveal a new polymorph of CaCO3, named CaCO3-VII, which is analogue of P21/c-l with different unit cell parameters. Enthalpies and Gibbs energies of aragonite-II and CaCO3-VII are equal within the DFT error. On compression CaCO3-VII became more energetically favourable and in experiments we observe transformation of aragonite-II to CaCO3-VII on compression.

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[*] Speaker

Preliminary data on the real perovksite (CaTiO3) phase diagram

François Guyot * [1], Lucas Maurice [2], Gaston Garbarino [3], Marion Harmand [4], Mohamed Mezouar [5], Francesca Miozzi [6], Guillaume Morard [1], A. Ravasio [7], Guillaume Fiquet† [4]

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The high-pressure *Pbnm*-perovskite structure of MgSiO3 is the most abundant mineral in the Earth's mantle. At pressure exceeding 120 GPa at high-temperature, a post-perovskite transition to a *Cmcm*-CaIrO3-structure of MgSiO3 has been shown by several authors. The same transition has been described in numerous other perovskite-structured compounds but a significant diversity of phases and transition paths have been reported in literature. Even iron and aluminium bearing MgSiO3 perovskites do not have a simple transition from *Pbnm*-perovskite to *Cmcm*-CaIrO3 showing intermediate phases often yet poorly understood.

In order to get a better insight on the different possible transition regimes in the complex silicate perovskite system, we have investigated the transformations at high pressure and high temperature of the actual perovskite mineral, CaTiO3. Moreover, as this compound already crystallizes in a *Pbnm*-perovskite structure at 1 bar and 300 K, it might present post post perovskite transitions at lower pressures than in MgSiO3. We have thus carried out *in-situ* X-ray diffraction experiments at the ID27 beamline of the european synchrotron radiation facility using laser-heated diamond-anvil cells.

We have first obtained a 300 K equation of state up to 110 GPa in Neon pressure transmitting medium. The results are in good agreement with previous literature data up to 55 GPa (Guennou et al., 2010 *Physical Review B 82 (13), pp.134101*) but we observed a change in compression regime at 60 GPa. Below 60 GPa, upon laser heating, CaTiO3 transforms to the *Pm-3m-* cubic perovskite with a positive slope in pressure-temperature coordinates. If however the pressure

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*Speaker

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exceeds 60 GPa, a new phase appears which is not *Cmcm*-CaIrO3- but instead polytypes of *Pbnm*-perovskite and *Cmcm*-CaIrO3 structures which have already been reported in literature in the silicate perovskite system (*Tschauner et al., 2008, Amer. Mineral. (93) 533-539*). Then, at higher pressure, laser-heating experiments have been carried out up to 160 GPa, revealing a new structure which has not been identified yet. Implications of these results for the evolution of perovskite structure in terrestrial planets will be discussed with special emphasis on transition widths and slopes.

Kinetics Of Bridgmanite To (Mg0.86,Fe0.14)SiO3-Post-Perovskite. Towards A Better Comprehension Of The D” Layer.

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The radial seismic structure about 200 km above the core-mantle boundary is marked by a decreasing in seismic velocity gradients and defined the top of the region called D” seismic discontinuity (Bullen1950). Moreover, at this P/T conditions, Bridgmanite, the main lower mantle mineral, transforms into its high-pressure phase of (Mg,Fe)SiO3 post-perovskite(pPv). Indeed, the transition from Bridgmanite to (Mg0.86,Fe0.14)SiO3-Post-Perovskite (pPv) has received considerable interest due to their thermodynamic properties that seem to explain many of the seismic anomalies of the D” layer. Here, we investigate the kinetics of the Bridgmanite to pPv transition by time-series experiments in the Laser Heated Diamond Anvil Cell (LHDAC) conducted at the P02.2 beamline of the PETRA III synchrotron. Product phases and extent of transformation are monitored in-situ as a function of time at pressure and temperature ranging from 126.5 to 130.5 GPa and from 1600 to 2500 K, respectively. The data were analyzed with the Avrami model of nucleation and growth in order to

determine the properties of this phase transition. Apparent activation energy could be, for the first time, extracted (Ea≈238 kJ.mol-1). Moreover, based on our data, we will present two possible kinetic models that have important implications in constraining the dynamics and kinetics of the Bridgmanite to pPv transition at the D” layer P/T conditions.

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Effect of fO2 on water solubility in minerals around the 410 km discontinuity: Analysis using Raman spectroscopy

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The top of the transition zone of Earth's mantle (410-670 km) is marked by the olivine – wadsleyite phase transition. Olivine and wadsleyite are nominally anhydrous minerals (NAMs), but both may contain various amounts of water as hydroxyl. As a point defect, OH may play an important role on the physical and melting properties of the mantle around the 410 km discontinuity.
Our approach is to study the water partition between the different minerals in pyrolytic composition under water-saturated conditions. As oxygen fugacity is a key parameter on fluid speciation, it has been buffered in the experiments with the use of metal-oxide mixtures covering a wide range of redox conditions (Fe-FeO, Ni-NiO, and Re-ReO2). All the experiments were performed at the LMV, in a Kawai-type multi-anvil press around 13 GPa, between 1200 and 1400◦C, in double sealed capsules to prevent fluid loss. Samples have been analyzed with SEM and electron microprobe to study the minerals composition, and Raman spectroscopy for the water content (Bolfan-Casanova et al., 2014) (a).

The small grain size (50μm average for olivine and wadsleyite), the high water content, and the impossibility to get a proper double polishing due to samples fragility render the use of FTIR extremely difficult. Raman spectroscopy allowed us an easy mineral identification even on small grains ($< 5\mu$m), and has been used for water quantification. Standards with known water concentration were used to build a correlation with the integrated intensity of the water bands of wadsleyite of various composition (Fo89 and Fo100). The correlation used for olivine and clinoenstatite are from Bolfan-Casanova et al. (2014) (a).

Preliminary results show a wide range of water contents, mainly increasing with fO2, and decreasing with increasing temperature. We will also discuss the positive impact of the measurements dispersion for each sample phases on the final estimation precision, as crystal orientation has a strong effect on peaks intensities in Raman spectra.

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(a) Bolfan-Casanova N., Montagnac G. and Reynard B. (2014) Measurement of water contents in olivine using Raman spectroscopy. American Mineralogist 99, 149-156.

Structural changes in perylene from UV Raman spectroscopy up to 1GPa

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Vibrational properties and structural changes under pressure of a highly luminescent molecular organic crystal have been

investigated by ultraviolet resonant Raman spectroscopy with a 244-nm excitation. Resonant Raman modes of alpha-perylene crystal up to 1GPa were followed under hydrostatic pressure in an anvil cell with a sapphire window transparent to ultraviolet light. Nonlinear evolution of intra-molecular modes is induced by pressure. Abrupt shifts of Raman wavenumbers suggest structural and planar modifications of the molecules in the crystal. We interpret these shifts as a first-order phase transition to a lower volume of unit cell. The luminescence of perylene crystal is gradually modified as a consequence of these structural changes. The present experimental setup allows investigating with Raman spectroscopy very luminescent molecules involved in chemical reactions and molecular organic crystals under relatively high pressure (up to 1GPa).

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Acoustic velocities across the olivine – wadsleyite – ringwoodite transitions and the seismic signature of the 410 km mantle discontinuity

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The phase changes of olivine (Mg,Fe)2SiO4 to its high pressure polymorphs, wadsleyite and ringwoodite, have long been associated with the seismic discontinuities observed at 410 and 520 km depth in the Earth's mantle. The position and thickness of these discontinuities potentially provide basic constraints on the temperature, chemical composition and water content of the mantle. A common practice is to infer these properties by comparing seismic observations with modeled velocities from equilibrium phase relations and elastic moduli of the individual phases. Here, we directly measured the evolution of velocities across the olivine phase changes in order to investigate the transient, *i.e.* time-dependent, processes of the transformation. We developed an experimental method that combines *in situ* X-ray diffraction and ultrasonic interferometry to follow the elastic wave velocities as a function of reaction progress, with a time resolution of _˜ 30 s. The experiments were carried out on the 1000 t multi-anvil press of the ID-13D beamline of the APS synchrotron (Chicago, USA). Samples were sintered polycrystalline powders of olivine with XFe=0.10 and XFe=0.52 composition, that have been reacted in the stability field of wadsleyite or ringwoodite at 7-12 GPa and 1000-1200 K. Measurements show an unexpected decrease in shear waves velocity at the onset of reaction, followed by a steady increase that correlates with the percentage of transformation. This velocity anomaly is coupled with an increase in attenuation as observed from amplitudes of S-waves echoes. We relate this softening at the early stage of transformation to the presence of the intermediate spinelloid phase, as observed in the pseudo-martensitic reaction mechanism. This velocity profile may help to explain the

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sharpness ($<$ 6 km) and reflectivity of the 410 km discontinuity that have long been difficult to interpret from phase equilibria alone.

Pressure-induced phase transition of dioptase: Single-crystal X-ray diffraction and Raman spectroscopy

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Silicates, comprising more than 90% of the Earth's crust, are one of the most fundamental and widespread mineral groups, whose behaviours under pressure are of long-standing interest. The investigation of physical and chemical properties of silicates gives a key for the explanation of the corresponding behaviours and properties of the Earth's crust and mantle, and furthermore Cu-based silicates enjoy the attention of researchers working in the fields of geology and mineralogy. Here, we have studied the compressional behaviours of dioptase up to _˜20 GPa at room temperature. A pressure-induced phase transition was studied on single-crystal using synchrotron X-ray diffraction and Raman spectroscopy. Synchrotron X-ray diffraction was carried out at the 13 BMC beamline (GSECARS) of the Advanced Photon Source. By analyzing high pressure behaviours of aqueous silicate minerals, we come to the conclusion that the form of water molecules plays a key role in the elasticity of annular silicate minerals. Knowledge of dioptase crystal chemistry will contribute more broadly to the stability of hydrous silicates and the field of mineralogy.

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*Speaker

Evaporating rocky planets: Critical vaporization of MgSiO3

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Vaporization is an important process in Earth's earliest evolution during which giant impacts are through to have produced massive silicate atmospheres. As experimental data are very limited, little is known of the near-critical vaporization of Earth's major oxide components. We have performed novel ab initio molecular dynamics simulations of vapor-liquid coexistence in MgSiO3. The simulations, based on density functional theory, begin with a suitably prepared liquid slab embedded in a vacuum. During the dynamical trajectory in the canonical ensemble, we see spontaneous vaporization, leading eventually to a steady-state chemical equilibrium between the two coexisting phases. We locate the liquid-vapor critical point at 6600 K and 0.40 g/cm3. The critical temperature that we find is significnatly less than assumed in most hydrodynamic simulations of giant impacts (8800 K), suggesting that these simulations substantially underestimate vaporization. By carefully examining the trajectories, we determine the composition and speciation of the vapor. We find that vaporization is incongruent: the vapor is significantly enriched in O and depleted in Mg as compared with the bulk composition. Dominant vapor species are O2 and SiO; also present are greater amounts of SiO2 and free atoms than predicted by extrapolation of experimental data. These results will have important implications for our understanding of the initial chemistry of the Earth and Moon and the initial thermal state of the Earth.

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[*] Speaker

Posters: General Topics

History of Japan-U.S./High Pressure Mineral Physics Seminars: 1976 to 2012

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Under the auspices of the U.S.-Japan Cooperative Science Program between the U. S. National Science Foundation and the Japan Society for the Promotion of Science, the first U.S.-Japan joint seminar on High Pressure Research Applications in Geophysics was held in Honolulu, Hawaii, 5-8 July 1976 and was attended by 47 scientists. Originated as bilateral U.S.-Japan seminars on high-pressure research applications in geophysics by Murli Manghnani and Syun-iti Akimoto, this series continued at 5-year intervals under those auspices from 1976 to 1996 [1981 in Hakone, Japan 1986 in Turtle Bay, Hawaii, 1991 in Ise, Japan, and 1996 in Maui,Hawaii], with venues alternating between Hawaii and Japan. In the 21st century, as a result of growing international interest in high-pressure mineral physics, the seminar series was re-envisioned with a broader focus than the original US-Japan bilateral series. The first of the new meetings entitled "High Pressure Mineral Physics Seminars" [HPMP-6] took place in Verbania, Italy on August 26-31, 2002. More than 84 scientists from Asia, Australia, the Americas and Europe attended. HPMPS-7 took place in Matsushima, Japan on May 8-12, 2007 and was attended by 134 scientists from throughout the world. In this paper, we review this history culminating with the HPMPS-8 at Lake Tahoe, California in July 2012, which was held jointly with the Annual Meeting of COMPRES: Consortium for Materials Properties Research in Earth Sciences.

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*Speaker

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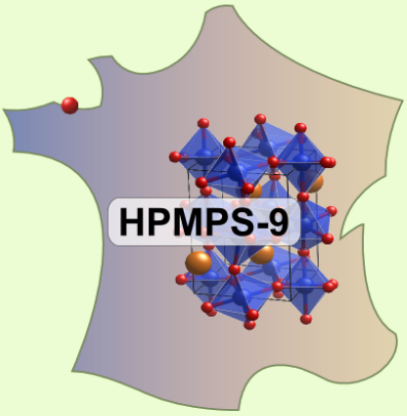

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