Workshop in Matsuyama, Japan November 4-7, 2015

# **The Earth's Mantle and Core**

Structure, Composition, Evolution



## Index

A Revised Chronology of the Inner Solar System <u>R. Brasser</u> , S. Mojzsis, S. Werner
Giant Impacts and Terrestrial Planet Formation <u>H. Genda</u>
Stable Isotope Evidence for Planetary Differentiation <u>A. Shahar</u> , S. Elardo, J. Labidi, W. Mao, R. Caracas, E. Schauble
Crystallization of Magma Oceans and Implications for Mantle Convection S. Labrosse, ChEd. Boukaré, M. Bouffard, A. Morison, Y. Ricard, P.J. Tackley, R. Deguen, T. Alboussière
<b>Early Evolution and Dynamics of Earth from a Molten Initial Stage</b> <u>D.L. Lourenço</u> , P.J. Tackley
Metal-Silicate Partitioning of Chlorine: Implications for the Origin of Terrestrial Missing Chlorine
H. Kuwahara, H. Gotou, N. Ogawa, A. Yamaguchi, T. Yagi, S. Sugita
Geochemical Evidence for the Temporal Evolution of the Mantle Redox State: Implications for the Volatile Outgassing <u>V. Stagno</u> , S. Aulbach
<b>Conductivity and Correlations at High Pressures in Fe and FeO</b> <u>R.E. Cohen</u> , P. Zhang, K. Haule
Core Neon M.A. Bouhifd, <u>A.P. Jephcoat</u> , D. Porcelli, S.P. Kelley
<b>Transport and Storage of Volatiles in the Mantle and Core</b> <u>E. Ohtani</u>
<b>From Star to Stone: What Really Makes an Exoplanet "Earth-like?"</b> <u>C.T. Unterborn</u> , W.R. Panero
Linear Analysis on the Onset of Thermal Convection of Highly Compressible Fluids with Variable Physical Properties: Implications for the Mantle Convection of Super-Earths <u>M. Kameyama</u>
Melting of Sahara 97072 Meteorite (EH3 Chondrite) at 12 GPa and VariableTemperatures <u>W. Du</u> , T. Irifune
Effective Temperature Condition in the Separation Process of the Core and Mantle <u>H. Ichikawa</u> , J. Hernlund, S. Labrosse, M. Kameyama

Effect of a Stratified Basal Magma Ocean on the Geodynamo ii

M. Laneuville, J. Hernlund, S. Labrosse, N. Guttenberg1	5
<sup>142</sup> Nd/ <sup>144</sup> Nd Isotope Systematics in the Early Earth and High-pressure Melting Experiments of Primitive Peridotite <u>N. Kondo</u> , T. Yoshino, K.N. Matsukage, T. Kogiso	6
<i>Ab initio</i> Electrical Resistivity of hcp Iron at Earth's inner Core Conditions <u>H. Dekura</u>	7
Hugoniot and Temperature Measurements of H <sub>2</sub> O up to 260 GPa Under Laser-driven Shock Loading	
<u>T. Kimura</u> , N. Ozaki, T. Sano, T. Okuchi, T. Sano, K. Shimizu, K. Miyanishi, T. Terai, T. Kakeshita, Y. Sakawa, R. Kodama	8
High-pressure <i>in situ</i> X-ray Laminography Using Diamond Anvil Cell <u>R. Nomura</u> , K. Uesugi	9
Phase Relations of FeH at Earth's Core Pressure <u>C. Kato</u> , K. Ohta, K. Hirose, Y. Ohishi	0
The Eutectic Liquid Composition in the Fe-Fe <sub>3</sub> S Binary System at the Core Pressure Range Y. Mori, S. Tateno, K. Hirose, G. Morard, Y. Ohishi	e 1
Some Thermodynamic Properties of Larnite (β-Ca <sub>2</sub> SiO <sub>4</sub> ) Constrained by High <i>T/P</i> Experiment and/or Theoretical Simulation <u>Z.H. Xiong</u> , X. Liu, S.R. Shieh	2
The Lower Mantle: A Seismological Perspective         B.L.N. Kennett.       2	3
Persistence of Strong Silica-Enriched Domains in the Earth's Lower Mantle J.W. Hernlund, C. Houser, M.D. Ballmer, R. Wentzcovitch, K. Hirose	4
<b>Discovery of New Iron Oxide Fe<sub>7</sub>O<sub>9</sub> and Its Solid Solution, (Mg,Fe<sup>2+</sup>)<sub>3</sub>Fe<sup>3+</sup><sub>4</sub>O<sub>9</sub></b> <u>R. Sinmyo, E. Bykova, S.V. Ovsyannikov, C. McCammon, I. Kupenko, L. Ismailova, L. Dubrovinsky</u>	5
Helium Diffusion in Mantle Minerals from First Principles J. Brodholt	6
<b>Modes of Slab Behavior: from the Transition Zone to the Mid-Lower Mantle</b> <u>C.R. Bina</u> , H. Čížková	7
Multiscale Seismic Tomography and Mantle Dynamics D.P. Zhao	8
Three-dimensional Analysis of Pore Effect on Composite Elasticity by Means of Finite Element Method <u>A. Yoneda</u>	9

Semi Analytical Model for the Effective Grain Size Profile in the Mantle of the Earth <u>A. Rozel</u> , G. Golabek, M. Thielmann, P.J. Tackley
The Relationship of Crystallographic Orientation between Perovskite and Post-Perovskite During Phase Transformation D. Yamazaki, M. Murakami, F. Xu, N. Hirao, Y. Seto
C. Houser, J. Hernlund, R. Wentzcovitch, J. Valencia-Cardona
Waveform Inversion for 3D Structure in D" <u>K. Kawai</u>
Adjacent High- and Low-Velocity Regions around the Western Edge of the Pacific Large-Low Shear Velocity Province S. Tanaka
<b>Technical Developments on Acoustic Emissions Monitoring at High Pressures</b> <u>T. Ohuchi</u> , X. Lei, Y. Higo, Y. Tange, T. Irifune
Creep Behavior of Fe-bearing Olivine under Hydrous Conditions <u>M. Tasaka</u> , M.E. Zimmerman, D.L. Kohlstedt
Stability Region of the (K, Na)AlSi <sub>3</sub> O <sub>8</sub> Hollandite Solid SolutionY. Zhou, T. Irifune, H. Ohfuji, T. Shinmei, W. Du
Direct Sound Velocity Measurements of Pyrolite Across the Mantle Transition Region S. Gréaux, T. Irifune, M. Nishi, Y. Higo, T. Inoue, T. Arimoto, Z. Liu
Effects of the Subducted Slab on Dynamics of the Lowermost Mantle <u>T. Kaneko</u> , T. Nakakuki
Single Crystal Elasticity of the Lower Mantle Minerals using Inelastic X-ray Scattering <u>H. Fukui</u> , A. Yoneda, A.Q.R. Baron
<b>Thermal Equation of State of MgSiO<sub>3</sub> Post-perovskite</b> <u>T. Sakai</u> , H. Dekura, N. Hirao
<b>Experimental Identification of a New Pyrite-type Hydroxide at Multimegabar Pressures</b> <u>M. Nishi</u> , Y. Kuwayama, J. Tsuchiya
<b>Technical Developments in High Temperature Generation with Sintered Diamond Anvils</b> <u>T. Arimoto</u> , T. Irifune, M. Nishi, Y. Tange, T. Kunimoto
<b>Over 3000°C Generation in Kawai-Cell Byboron-Doped Diamond Cylinder Heater</b> <u>L.J. Xie</u> , A. Yoneda, E. Ito
Properties of Liquid Iron Alloys under Extreme Conditions G. Morard, D. Andrault, D. Antonangeli, J. Siebert, F. Guyot, A.L. Auzende, O. Lord,

J. Bouchet, M. Harmand, B. Cochain, G. Garbarino, I. Kantor, R.Torchio, E. Boulard, M. Mezouar4	5
Liquid Iron Alloys with Hydrogen at Outer Core Conditions by First Principles K. Umemoto, K. Hirose	6
Core Liquids: Fact and Fiction <u>G. Helffrich</u>	7
<b>Crystallization of SiO<sub>2</sub> in Earth's Core after High-temperature Core Formation</b> <u>K. Hirose,</u> G. Morard, H. Ozawa, G. Helffrich, J. Hernlund	8
Linking Seismic Observations of Earth's Inner Core Boundary to Deeper Structure L. Waszek, A. Deuss, H. Godwin	9
Freezing and Melting above the Inner Core Boundary <u>M. Lasbleis</u> , J. Hernlund, S. Labrosse	0
Thermal Structure of the Inner Core Boundary in Numerical Dynamos <u>H. Matsui</u> 5	1
Lattice Preferred Orientation of Hcp-Iron Induced by Shear Deformation Y. Nishihara, T. Ohuchi, T. Kawazoe, G. Maruyama, Y. Higo, K. Funakoshi, Y. Seto	2
View and Perspectives on the Lower Mantle from Geo-neutrinos S.T. Dye	3
<b>Geo-neutrino Measurement with KamLAND and Future Prospects</b> <u>H. Watanabe</u>	4
Core and Mantle Compositions: Neutrino Geophysics Insights <u>W.F. McDonough</u>	5

#### A Revised Chronology of the Inner Solar System

<u>R. Brasser</u><sup>1</sup>, S. Mojzsis<sup>2</sup>, S. Werner<sup>3</sup>

## <sup>1</sup>ELSI, <sup>2</sup>University of Colorado, Boulder, <sup>3</sup>University of Oslo Corresponding author's email address: brasser@elsi.jp

Hadean (pre-3900 Ma) terrains are the oldest and most heavily cratered on the Moon, Mercury and Mars [1], the latter two having crater densities comparable to the ancient highlands of the Moon [1]. All three bodies were heavily bombarded during the first 600 million years of the Solar System. Post-formation accretion has been suggested to follow a "Sawtooth" [2] intensity profile, but its precise timing remains elusive. From zircons and apetite crystals of lunar samples, Martian and Vestan meteorites, NASA Curiosity isotope age measurements [3] and an updated Martian crater chronology [4], the inner solar system likely experienced another intense episode of bombardment long after the formation of the terrestrial planets [5]. The second of these has been dubbed the lunar cataclysm or Late Heavy Bombardment (LHB). Traditionally the peak bombardment was thought to occur at 3.95 Ga, and recently the start has been pushed to 4.1 Ga[2], the supposed age of Nectaris basin. However, recent evidence shows Nectaris is older[6], casting its timing into doubt. From the resetting and fracture ages of zircons on the Moon, Mars and Vesta, we determine the onset of the LHB to be near 4.3 Ga, after which the bombardment declined monotonically. We discuss the implications of this and construct a new timeline for the evolution of the inner solar system.

<u>References</u>. [1] Werner, S. C. (2014): *Earth and Planetary Science Letters*, **400**, 54; [2] Morbidelli, A., Marchi, S., Bottke, W.F., and Kring, D.A. (2012): *Earth and Planetary Science Letters*, **355**, 144; [3] Farley, K. A. et al. (2014): *Science*, **343**, 1247; [4] Werner, S. C., Ody, A., and Poulet, F. (2014): *Science*, **343**, 1343; [5] Bottke, W.F., et al. (2012): *Nature*, **485**, 78; [6] Fischer-Godde, M., and Becker, H. (2011): *Lunar and Planetary Science Conference*, **42**, 1414.

#### **Giant Impacts and Terrestrial Planet Formation**

#### H. Genda

Earth-Life Science Institute, Tokyo Institute of Technology Corresponding author's email address: genda@elsi.jp

There are wide varieties of physical and chemical states among terrestrial planets in our solar system, such as their sizes, orbits, spin states (also presence of moon), the amount and composition of atmosphere, the presence of ocean and life etc. How have these varieties been built? Although the long-term evolutions on each planet are also important, here we focus on the formation stage of the terrestrial planets. This is because very energetic events occur during the planet formation, such as the collisions among planetesimals [1, 2] and protoplanets [3, 4].

Especially, several tens of Mars-sized protoplanets collide with each other to form the terrestrial planets during the last stage of the terrestrial planet formation [5, 6, 7]. This stage is called the giant impact stage. Such energetic collisions should have a great influence on the various features of the terrestrial planets. For example, giant impacts are responsible for the creation of the Moon [3,8] and the Martian satellites [9], and planets with extremely large cores such as Mercury [10]. Giant impacts also affect volatile budget in terrestrial planets [11, 12], and leads to magma ocean [13]. Cooling of magmaocean and escape of water vapor results in difference in water content on Earth and Venus [14].

Even in extrasolar planetary systems, giant impact events are thought to be common. Recently, thanks to infrared space telescopes such as Spitzer and AKARI, tens of warm debris disks around solar-type (FGK) stars with ages of  $10^7-10^8$  yearshave been reported [15,16]. These warm debris disks are estimated to be located roughly 1 AU to several AU from the central stars, which corresponds to the terrestrial planet region in the solar system. Based on their stellar ages and locations of the debris disks, the relation between these warm debris disks and giant impact events has recently been discussed [17, 18, 19].

<sup>&</sup>lt;u>References.</u> [1] Benz & Asphaug. (1999): *Icarus*, 142, 5–20; [2] Genda, H. et al. (2015): *Icarus*, 262, 58–66; [3] Canup. (2004): *Annu. Rev. Astron. Astrophys*, 42, 441–475; [4] Genda, Kokubo and Ida. (2012): *Astrophys. J*, 744, 137 (8pp); [5] Chambers. (2001): *Icarus*, 152, 205–224; [6] Kokubo and Genda. (2010): *Astrophys. J. Lett*, 714, L21–L25; [7] Walsh, M. et al. (2011): *Nature*, 475, 206–209; [8] Genda and Abe. (2003): *Earth Planets Space*, 55, 53–57; [9] Citron, Genda and Ida. (2015): *Icarus*, 252, 334–338; [10] Benz. (2007): *Space Sci. Rev*, 132, 189–202. [11] Genda and Abe. (2003): *Icarus*, 164, 149–162; [12] Genda and Abe.(2005): *Nature*, 433, 842–844; [13] Tonks and Melosh. (1992): *Icarus*, 100, 326–346; [14] Hamano, Abe and Genda. (2013): *Nature*, 497, 607–610; [15] Zuckerman, Rhee, Song and Bessell. (2011): *Astrophys. J*, 732, 61 (19pp); [16] Fujiwara, Ishihara, Onaka, et al. (2013): *Astron. Astrophy*, 550, A45; [17] Jackson and Wyatt (2012): *Mon. Not. R. Astron. Soc*, 425, 657–679; [18] Melis, Zuckerman, Rhee, et al. (2012): *Nature*, 487, 74–76; [19] Genda, Kobayashi & Kokubo. (2015): *Astrophys. J*, 810, 136 (8pp).

#### **Stable Isotope Evidence for Planetary Differentiation**

<u>A. Shahar<sup>1</sup></u>, S. Elardo<sup>1</sup>, J. Labidi<sup>1</sup>, W. Mao<sup>2</sup>, R. Caracas<sup>3</sup>, E. Schauble<sup>4</sup>

## <sup>1</sup>Geophysical Laboratory, Carnegie Institution of Washington, <sup>2</sup>Stanford University, <sup>3</sup>Ecole Normal Superieure de Lyon, <sup>4</sup>University of California Los Angeles Corresponding author's email address: ashahar@ciw.edu

The differentiation of planetesimals occurred at high temperature, varying pressure, varying oxygen fugacity and on bodies with varying compositions. As increasing knowledge points to the Earth and other terrestrial bodies being formed by already differentiated planetesimals it is essential that we understand what these planetesimals looked like in order to fully understand how the Earth and other terrestrial planets formed. In this study we focus on what we can learn about the differentiation of planetesimals from stable isotope ratios.

During the differentiation process, the iron molten metal will alloy with other elements on its route to the center of the planetary body. Which elements it bonds with will be a function of the conditions attending the core formation. For example, at high temperature under reducing conditions Si is likely to alloy with iron, however, in more oxidizing conditions sulfur is likely to enter the metal. Determining which elements reside in planetary interiors requires indirect methods such as high pressure and temperature experimental studies. The main candidates considered are carbon, sulfur, oxygen, silicon and hydrogen.

We contend that by determining the equilibrium stable isotopic fractionation between metal and silicate we can provide an independent constraint on the composition of a planetary body and specifically address the likelihood of each light element in the core. The nature of the light element in an Fe-Ni core is directly related to the mode of formation, for example, whether differentiation occurred at high pressure or low pressure, the redox conditions present, or the composition of the melt. Through high pressure and temperature experiments we can systematically probe these variables and determine which are the most important in influencing the stable isotope ratios found in natural samples today.

#### **Crystallization of Magma Oceans and Implications for Mantle Convection**

<u>S. Labrosse</u><sup>1</sup>, Ch.-Ed. Boukaré<sup>1</sup>, M. Bouffard<sup>1</sup>, A. Morison<sup>1</sup>, Y. Ricard<sup>1</sup>, P.J. Tackley<sup>2</sup>, R. Deguen<sup>1</sup>, T. Alboussière<sup>1</sup>

<sup>1</sup>ENS de Lyon, Univ. Lyon-1, France, <sup>2</sup>ETH Zürich Corresponding author's email address: Stephane.labrosse@ens-lyon.fr

Classical models of magma ocean assumed that crystallization proceeded upwardly from the bottom because the pressure dependence of the liquidus is steeper than the liquid isentrope at moderate pressure. Recent studies on high pressure melting of silicate show that this may not have been the case and crystallization could have started from the mid-mantle [1, 2, 3]. The dynamics and evolution following that initial crystal formation depends on the relative densities of solids and liquids and of the density stratification in the solid resulting from crystallization. It is likely that a significant upper part of the magma ocean fractionally crystallized from the bottom. Upon fractional crystallization, the liquid becomes enriched in FeO and so does the solid that forms from it, leading to an unstably stratified solid mantle. If crystallization completes before convection starts in the solid, its temperature at the end of crystallization follows the solidus whose pressure and composition dependence make it super-isentropic. Therefore, both composition and temperature stratifications in the mantle following a bottom-up crystallization contribute in producing a Rayleigh-Taylor instability leading to an overturn of the solid mantle [4,5]. This overturn occurs very fast and leads to a stably stratified mantle with hot and FeO-poor material overlying cold and FeO-rich mantle. Thermal convection then resumes by cooling at the surface of the solid mantle but has to overcome the initial stratification. Using a mantle convection code (StagYY [6]) in which the initial conditions are those predicted for a bottom-up magma ocean crystallization, we study the impact of various parameters (depth of initial crystallization, partition coefficient of FeO, Rayleigh number) on the ability of mantle convection to erase the initial stratification produced by magma ocean overturn.

<u>References</u>. [1] Fiquet, G. et al. (2010): *Science*, **329**, 1516–1518; [2] Thomas, C.W. et al. (2012): *J. Geophys. Res*, **117**, B10206; [3] Boukaré, C.-E., Ricard, Y., Fiquet, G. (2015): *J. Geophys. Res*, **120**,6085–6101; [4] Hess, P.C. and Parmentier, E.M. (1995): *Earth Planet. Sci. Lett*, **134**, 501–504; [5] Elkins-Tanton, L.T., Parmentier, E.M. and Hess, P.C. (2003): *Meteoritics Planet. Sci*, **38**, 1753–1771; [6] Tackley, P.J. (2008): *Phys. Earth Planet. Inter*, **171**, 7–18.

#### Early Evolution and Dynamics of Earth from a Molten Initial Stage

#### D.L. Lourenço, P.J. Tackley

Institute of Geophysics, Department of Earth Sciences, ETH Zürich, Switzerland Corresponding author's email address: diogo.lourenco@erdw.ethz.ch

It is now well established that most of the terrestrial planets underwent a magma ocean stage during their evolution. On Earth, it is probable that at the end of accretion, giant impacts like the Moon-forming impact, together with other sources of heat, melted a substantial part of the mantle.

Considerable research has been done on magma oceans using simple 1-D models [e.g.: 1, 2, 3]. However, some aspects of the dynamics may not be adequately addressed in 1-D and require the use of 2-D or 3-D models. Moreover, new developments in mineral physics that indicate that melt can be denser than solid at high pressures [e.g.: 4] can have very important impacts on the classical views of the solidification of magma oceans [5].

The goal of our study is to understand and characterize the influence of melting on the long-term thermo-chemical evolution of rocky planet interiors, starting from an initial molten state (magma ocean). Our approach is to model viscous creep of the solid mantle, while parameterizing processes that involve melt as previously done in 1-D models, including melt-solid separation at all melt fractions, the use of an effective diffusivity to parameterize turbulent mixing, coupling to a parameterized core heat balance and a radiative surface boundary condition. These enhancements were made to the numerical code StagYY [6].

We will present results for the evolution of an Earth-like planet from a molten initial state to present day, while testing the effect of uncertainties in parameters such as melt-solid density differences, surface heat loss and efficiency of turbulent mixing. Our results show rapid cooling and crystallization until the rheological transition then much slower crystallization, large-scale overturn well before full solidification, the formation and subduction of an early crust while a partially-molten upper mantle is still present, transitioning to mostly-solid-state long-term mantle convection and plate tectonics or an episodic-lid regime.

<sup>&</sup>lt;u>References</u>:[1] Abe, Y. (1997): *PEPI*, **100**, 27-39; [2] Solomatov, V. S. (2007): *Treat. Geophys*, **9**, 91-120; [3] Elkins-Tanton, L. T. (2008): *EPSL*, **271**, 181-191; [4] de Koker, N., Karki, B. B., Stixrude, L. (2013): *EPSL*, **361**, 58-63; [5] Labrosse, S, Hernlund, J. W, Coltice, N. (2007): *Nature*, **450**, 866-869; [6] Tackley, P. J. (2008): *PEPI*, **171**, 7-18.

## Metal-Silicate Partitioning of Chlorine: Implications for the Origin of Terrestrial Missing Chlorine

H. Kuwahara<sup>1</sup>, H. Gotou<sup>2</sup>, N. Ogawa<sup>3</sup>, A. Yamaguchi<sup>3</sup>, T. Yagi<sup>4</sup>, and S. Sugita<sup>1,4</sup>

<sup>1</sup>Departmentof Complexity Science and Engineering, University of Tokyo <sup>2</sup>Institute for Solid State Physics, University of Tokyo <sup>3</sup>Atmosphere and Ocean Research Institute, University of Tokyo <sup>4</sup>Deptartment of Earth and Planetary Science, University of Tokyo Corresponding author's email address: kuwahara@astrobio.k.u-tokyo.ac.jp

The chlorine abundance of the bulk silicate Earth may be greatly depleted relative to the prediction based on various types of primitive materials, such as chondrites [1]. There are two hypotheses for this depletion of terrestrial chlorine; Incorporation into the Earth's core and a collisional erosion of primordial hydrosphere. Here we experimentally examine the possibility of the former case. Specifically, the metal-silicate partitioning of chlorine in a magma ocean is investigated.

In this study, we experimentally determined the metal-silicate partition coefficient of chlorine as functions of pressure and temperature. Starting materials were prepared from a mixture of high-purity oxides (SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, CaO, MgO, FeO) and metal (Fe, FeS). The relative abundances of each component in the silicate portion were assumed to be chondrites. Chlorine was added to the mixture as FeCl<sub>2</sub>. The starting materials were enclosed in either a graphite capsule or a single crystal MgO capsule. The experiments were performed at 4-23 GPa and 1923-2673 K using the multi-anvil press. The chemical compositions of recovered samples were analyzed by wavelength-dispersive electron microprobe.

Our experimental results show that (1) chlorine is highly lithophile, (2) the metal-silicate partition coefficient of chlorine increases with increasing temperature, and decreases with increasing pressure. Based on the experimental results and thermodynamic consideration, we estimated the metal-silicate partitioning of chlorine at the base of a magma ocean which becomes deeper as accretion proceeds. The *P*-*T* conditions at the base of a magma ocean were assumed to be the same as the peridotite melting curve. Calculation results show that the metal-silicate partition coefficients of chlorine at the base of a magma ocean are much lower than the required value proposed by Sharp & Draper [1]. Thus, Earth's core is unlikely to be the origin of terrestrial missing chlorine. Given that the fluid-melt partition coefficient of chlorine is  $\sim 10$  [e.g., 2], chlorine is likely to be partitioned into primordial hydrosphere. If this is the case, terrestrial missing chlorine may require an extensive loss of primordial atmospheres and oceans during the main-accretion phase.

<u>Reference</u>. [1] Sharp, Z. D. and Draper, D. S. (2013): *EarthPlanet. Sci. Lett*, **369-370**, 71-77; [2] Metrich, N. et al. (2001): *Journal of Petrology*, **42**, 1471-1490.

## Geochemical Evidence for the Temporal Evolution of the Mantle Redox State: Implications for the Volatile Outgassing

V. Stagno<sup>1,2</sup>, S. Aulbach<sup>3</sup>

<sup>1</sup>Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo 152-8550, Japan <sup>2</sup>Geodynamic Research Center, Ehime University, Matsuyama, Japan <sup>3</sup>Goethe Universität, Frankfurt, Germany

The oxidation state (fo<sub>2</sub>) of the interior of Earth has modulated the extraction of volatiles from depth and their redistribution to the shallower portions of the planet and, eventually, to the hydrosphere and atmosphere through time. During core formation and crystallisation of the early-Earth from a magma ocean, the reducing  $f_{O2}$  likely buffered by the equilibrium between the primitive silicate melt and the percolating Fe metal promoting immobility of C-O-H gaseous species; whereas presently  $f_{O2s}$  between -1 and 0 log units (FMQ) as recorded by mid-ocean ridges basalts (MORBs) can mobilize large amount of volatiles from depths of the lower/upper mantle.

To date, several studies have interpreted similar oxidised conditions for mantle-derived melts (komatiites, picrites, and basalts) from  $\sim 3800$  Ma as evidence that the mantle  $f_{02}$  has attained its present value shortly after core formation and remained relatively constant over time. Whether this increase was gradual or not, at least up to the Hadaean, remains debated and strongly dependent on what mechanisms operated.

We use the V/Sc ratio of preserved Archean orogenic and mantle eclogites that have low-pressure protoliths separated from a spinel peridotite source to unravel the redox history of the convecting mantle. The mantle oxidation state in the Archaean convecting mantle and possible implications for the speciation of volatiles is reviewed based on geochemical data combined with thermodynamic predictions of the variation of fo2 as function of depth, temperature and bulk composition.

This has several consequences such as, (1) the locus of a volatile-bearing peridotite solidus and the composition of fluids/melts that formed along the mantle adiabat; (2) redox melting as a precursor to continental rifting during which carbonatitic to carbonate-silicate melts might have been the first magmas to be erupted, and (3) the increase in atmospheric  $CO_2$  accompanied by first whiffs of oxygen.

Reference.[1] Li and Lee. (2004): EPSL, 228, 483-493; [2] Scaillet and Gaillard. (2011): Nature, 480, 48-49.

#### **Conductivity and Correlations at High Pressures in Fe and FeO**

<u>R.E. Cohen<sup>1,2</sup></u>, P. Zhang<sup>1,3</sup>, K. Haule<sup>4</sup>

<sup>1</sup>Extreme Materials Initiative, Geophysical Laboratory, Carnegie Institution for Science, Washington, D.C. USA
<sup>2</sup>Department für Geo-und UmweltwissenschaftenLudwig-Maximilians-Universitaet, Munich, Germany
<sup>3</sup>Department of Physics, Xi'An Jiaotong University, Xi'an, Shaanxi, China
<sup>4</sup>Deptartment of Physics, Rutgers University, USA
Corresponding author's email address: rcohen@carnegiescience.edu

Under pressures in the Earth, iron in minerals behaves very differently from simple elements, such as magnesium, even though  $Fe^{2+}$  and  $Mg^{2+}$  easily substitute for each other at low pressures. I will discuss the behavior of FeO and Fe under high pressures and temperatures using modern electronic structure methods. FeO is an insulator at ambient conditions, but at high pressures and temperatures we found it becomes a metal [1]. We are investigating these properties using a method beyond the standard model, density functional theory (DFT), for electronic structure. We are using self-consistent DFT/Dynamical Mean Field Theory (DMFT)[2], which includes quantum and thermal fluctuations, multiplets, and all-orders of local electronic correlations. We find that electron correlations are important even in the generation of Earth's magnetic field. Earth's magnetic field was believed to arise from thermal convection of molten iron allov in Earth's outer core, but density functional theory (DFT) calculations suggested that the conductivity of iron is too high to support thermal convection[3-6], so that new geodynamo models were being developed[7, 8]. The DFT computations for resistivity were based on the scattering of electrons off of atomic vibrations, or electron-phonon (e-p) scattering. We applied self-consistent density functional theory plus dynamical mean-field theory (DFT+DMFT) [2] to iron and found that at high temperatures electron-electron (e-e) scattering is comparable to the e-p scattering, bringing theory into agreement with experiments and solving the transport problem in Earth's core, consistent with the conventional thermal geodynamo[9]. How electron correlations change with pressure, and how this affects material properties, will be discussed. This work is supported by the US National Science Foundation and the ERC Advanced grant ToMCaT.

<u>References</u>. [1] K. Ohta, R.E. et al. (2012): *Phys. Rev. Lett*, 108; [2] K. Haule, C. H. Yee, and K. Kim. (2010): *Phys. Rev. B*, 81; [3] X. Sha and R. E. Cohen, J. (2011): *Phys. Cond. Matt*, 23, 075401; [4] N.de Koker, G. Steinle-Neumann, and V. Vlcek. (2012): *Proc Natl Acad Sci USA*, 109, 4070; [5] H. Gomi, K. Ohta, K. Hirose, S. Labrosse, R. Caracas, M. J. Verstraete, and J. W. Hernlund. (2013): *Phys. Earth Planet. Int*, 224, 88; [6] M. Pozzo, C. Davies, D. Gubbins, and D. Alfe. (2012): *Nature*, 485, 355; [7] B. Buffett. (2012): *Nature*, 485, 319; [8] P. Olson. (2013): *Science*, 342, 431; [9] P. Zhang, R. E. Cohen, and K. Haule. (2015): *Nature*, 517, 605.

#### **Core Neon**

M. A. Bouhifd<sup>1,</sup> <u>A.P. Jephcoat</u><sup>2</sup>, D. Porcelli<sup>3</sup>, S.P. Kelley<sup>4</sup>

 <sup>1</sup>Laboratoire Magmas et Volcans, Université Blaise Pascal, CNRS UMR 6524, OPGC-IRD, 5 Rue Kessler, 63038 Clermont-Ferrand Cedex, France
 <sup>2</sup>Institute for Study of the Earth's Interior, Okayama University, Yamada 827, Misasa, Tohaku, Tottori 682-0193 Japan
 <sup>3</sup>University of Oxford, Department of Earth Sciences, Parks Road, Oxford, OX1 3AN, UK
 <sup>4</sup>Department of Environment, Earth and Ecosystems, Open University, Milton Keynes MK7 6AA, UK
 Corresponding author's email address: andyj@okayama-u.ac.jp

Noble gases have long been the archetypal tracers of mantle processes [1]. Their inertness combined with an array of 23 stable isotopes has led to a wealth of mantle diagnostic studies impinging on primordial origins and evolution, trapping history, recycling, radiogenic production, and mantle reservoir interactions. The incompatibility of noble gases has dominated the thinking on mantle evolution coupled with outgassing to the atmosphere. The mantle likely remains the dominant source of trapped inventory to the present day. Here we consider the possibilities of a core component on noble gas budgets, and the contributions possible with the context of limited core-mantle exchange.

The partitioning of neon between liquid silicate and molten iron-rich metal under conditions of Earth's early core formation to 16 GPa and ~3000K was simulated in a diamond-anvil cell under neon-rich conditions. Ultraviolet laser ablation mass spectrometric methods were used to analyse recovered samples. We find, as in the case of helium previously [2], that the metal phase can contain significant, non-zero quantities of neon.

We compare the relative and absolute partitioning of Ne and He in these experiments. In the context of the whole Earth, the possibilities of a core signature on noble gas segregation during accretion or an imprint on the mantle noble gas systematics as observed today are discussed.

<u>References</u>. [1] Hilton, D.R & Porcelli, D. (2014): *Treatise in Geochemistry 2<sup>nd</sup> Edition*, Vol. 3. (Turekian KK, Holland HD, Eds.) 327-353, Oxford: Elsevier Science; [2] Bouhifd, M.A., Jephcoat, A.P., Heber, V.S., Kelley, S.P. (2013): *Nature Geosci*, **6**, 982-986

#### **Transport and Storage of Volatiles in the Mantle and Core**

#### E. Ohtani

Department of Earth Science, Graduate school of Science Tohoku University, Sendai, 980-8578, Japan

Corresponding author's email address: ohtani@m.tohoku.ac.jp

Materials in the surface of the Earth including volatiles can penetrate into the deep Earth through slab subduction. The transition zone has a water storage capacity of approximately 0.5–1 wt% due to a high water solubility in wadsleyite and ringwoodite, which are the major constituents in the transition zone. Water has significant effects on the boundaries of the phase transformations of the mantle minerals, and can explain some topography of the 410 and 660 km seismic discontinuities [1]. Recent discovery of hydrous ringwoodite containing water about 1 wt. % [2] and hydrous phase Egg AlSiO<sub>3</sub>OH [3] as inclusions in diamond strongly favors existence of the hydrous transition zone, a major water reservoir in the Earth's interior.

We estimated the existence of the density crossover between magma and minerals at the base of the upper mantle and the core-mantle boundary region [4, 5]. The hydrous melt formed by dehydration melting can also be gravitationally stable at these regions [6]. Dehydration of the wet transition zone can generate wet plumes originating at the base of the upper mantle. We proposed a big mantle wedge model [7] caused by dehydration from the stagnant slabs, which can explain the seismic tomographic model beneath northeast China. When subducting stabs penetrate into the lower mantle, dehydration melting can occur also below the transition zone [8].

We discovered a hydrous-phase AlOOH-MgSiO<sub>2</sub>(OH)<sub>2</sub> solid solution as the reaction product of garnet and water [9], and clarified that the end-member hydrous phase d-AlOOH is stable up to the base of the lower mantle [10]. Recently an end-member phase MgSiO<sub>2</sub>(OH)<sub>2</sub>, named as hydrous phase H, MgSiO<sub>2</sub>(OH)<sub>2</sub> was also reported [11, 12]. We revealed that stability of the end member phase H and phase d-H solid solution up to the base of the lower mantle [13, 14]. The dehydration melting could occur at the base of the lower mantle providing a potential origin of the ultra-low velocity zone at the core-mantle boundary. When this hydrous phase or hydrous magma contacts with metallic iron of the core at the core-mantle boundary, hydrogen is likely to be dissolved into the outer core.

Measurement of the sound velocity of FeH at high pressure by using IXS (Inelastic X-ray Scattering) revealed that the seismic velocity and density of the core can be explained by existence of maximum 0.23(6) wt. % H in the core [15], which indicates that the core is undersaturated in hydrogen. Therefore, the core is currently a sink of hydrogen at the base of the lower mantle.

References. [1] Ohtani E. and Litasov K. (2006): *Rev. Mineral. Geochemistry*, vol.62, Chapter **17**, 397-420; [2] Pearson, D.G. et al. (2010): *Nature*, 507, 7491, 221; [3] Wirth, R. et al. (2007): *Earth Planet. Sci. Lett*, **259**, 384–399; [4] Ohtani E. (1983): *Phys. Earth Planet. Inter*, **33**, 12-25; [3] Ohtani E.(1985): *Phys. Earth Planet. Inter*, **38**, 70-80; [5] Ohtani E. & Maeda, M. (2001): *Earth and Planetary Science Letters*, **193**, 69-75; [6] Sakamaki, T. et al. (2006): *Nature*, **439**, 192-194; [7] D. Zhao & Ohtani E. (2009): *Gondwana Research*,16, Issues **3-4**, 401-413; [8] Schmandt et al. (2014): *Science*, 344, 1265; [9] Suzuki, A.et al. (2000): *Phys. Chem. Mineral*, 27, 689-693; [10] Sano A. et al. (2008): *Geophysical Research Letters*, **35**(3), L03303; [11] Tsuchiya, J.(2013): *Geophys. Res. Lett*, **40**, 4570–4573; [12] Nishi, M. et al. (2014): *Nat. Geosci*, 7, 224–227; [13] Ohira I. et al. (2014): *Earth and Planetary Science Letters*, **41**, 23, 8283-8287; [15] Shibazaki Y. et al. (2012): *Earth and Planetary Science Letters*, **313-314**, 79-85.

#### From Star to Stone: What Really Makes an Exoplanet "Earth-like?"

## C.T. Unterborn, W.R. Panero

## School of Earth Sciences, The Ohio State University Corresponding author's email address: unterborn.1@osu.edu

Plate tectonics have operated on Earth for a majority of its lifetime. Tectonics regulates atmospheric carbon and creates a planetary-scale water cycle, and is a primary factor in the Earth being habitable. While the mechanism for initiating tectonics is unknown, as we expand our search for habitable worlds, understanding which planetary compositions produce planets capable of supporting *long-term* tectonics is of paramount importance. On Earth, this sustentation of tectonics is a function of both its structure and composition. Currently, however, we have no method to measure the interior composition of exoplanets. In our Solar system, though, Solar abundances for refractory elements mirror the Earth's to within ~10%, allowing the adoption of Solar abundances as proxies for Earth's. It is not known, however, whether this mirroring of stellar and terrestrial planet abundances holds true for other star-planet systems without determination of the composition of initial planetesimals via condensation sequence calculations. Currently, all code for ascertaining these sequences are commercially available or closed-source. We present, then, the open-source Arbitrary Composition Condensation Sequence calculator (ArCCoS) for converting the elemental composition of a parent star to that of the planet-building material as well as the extent of oxidation within the planetesimals.

These data allow us to constrain the likelihood for one of the main drivers for plate tectonics: the basalt to eclogite transition subducting plates. Unlike basalt, eclogite is denser than the surrounding mantle and thus sinks into the mantle, pulling the overlying slab with it. Without this higher density relative to the mantle, plates stagnate at shallow depths, shutting off plate tectonics. Using the results of ArCCoS as abundance inputs into the MELTS and HeFESTo thermodynamic models, we calculate phase relations for the first basaltic crust and depleted mantle of a terrestrial planet produced from a given stellar composition. We find that for many stellar systems, the basalt-eclogite transition does not increase plate density enough relative to the mantle. Even should these planets initiate plate tectonics, the plate will stagnate in the shallow mantle, shutting off tectonics and produce a planet not habitable to life as we know it. Here, we present an outline for estimating the likelihood of an extrasolar planet being "Earth-like" and potentially habitable as well as preliminary results for various planetary systems.

## Linear Analysis on the Onset of Thermal Convection of Highly Compressible Fluids with Variable Physical Properties: Implications for the Mantle Convection of Super-Earths

## M. Kameyama

Geodynamics Research Center, Ehime University, Matsuyama, Japan Corresponding author's email address: kameyama@sci.ehime-u.ac.jp

A series of our linear analysis on the onset of thermal convection wasapplied to that of highly compressible fluids in a planar layer whose thermal conductivity and viscosity vary in space, in order to study the influences of spatial variations in physical properties expected in themantles of massive terrestrial planets. The thermal conductivity and viscosity are assumed to exponentially depend on depth and temperature, respectively, while the variations in thermodynamic properties (thermal expansivity and reference density) with depth are taken to be relevant for the super-Earths with 10 times the Earth's.

Our analysis demonstrated that the nature of incipient thermalconvection is strongly affected by the interplay between the adiabatic compression and spatial variations in physical properties of fluids.Owing to the effects of adiabatic compression, a ``stratosphere" canoccur in the deep mantles of super-Earths, where a vertical motion isinsignificant.An emergence of "stratosphere" is greatly enhanced by the increase inthermal conductivity with depth, while it is suppressed by the decrease in thermal expansivity with depth.In addition, by the interplay between the static stability and strongtemperature-dependence in viscosity, convection cells tend to beconfined in narrow regions around the "tropopause" at the interfacebetween the "stratosphere" of stable stratification and the "troposphere" of unstable stratification.

We also found that, depending on the variations in physical properties, two kinds of stagnant regions can separately develop in the fluid layer. One is well-known ``stagnant-lids" of cold and highly viscous fluids, and the other is ``basal stagnant regions" of hot and less viscousfluids. The occurrence of ``basal stagnant regions" may imply that convectingmotions can be insignificant in the lowermost part of the mantles of massive super-Earths, even in the absence of strong depth-dependence inviscosity.

#### Melting of Sahara 97072 Meteorite (EH3 Chondrite) at 12 GPa and Variable Temperatures

<u>W.  $Du^{1,2}$ </u>, T. Irifune<sup>1,2</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University <sup>2</sup>Earth-Life Science Institute, Tokyo Institute of Technology Corresponding author's email address: wei\_du@sci.ehime-u.ac.jp

The accretion and early differentiation of the Earth is the starting point of earth history.Because of their isotopically identical to the Earth, enstatitechondrites(E-chondrite) have been proposed as a model for the chemical composition of the bulk Earth [1, 2].However, the most recent study on silicon isotope by Fitoussi and Bourdon (2012)[3] argued that to get consistent with the isotopic composition of bulk silicate Earth, the Earth's core need to contain as much as 28 wt% Si, which is then not consistent with the density deficit deduced from seismic velocities.Start from an estimate of the bulk earth composition to evaluate the conditions of core-mantle differentiation by simple melting experiments at high temperature and relatively high pressure could be an alternative strategy to evaluate the proposed models for the Earth's formationand its early differentiation.

In this study, we present the first serial of melting experiments on Sahara 97072 meteorite, an EH3 chondrite with least metamorphosed [4] at relatively high pressure (12 GPa) and different temperatures (1000-2000°C), to compare the liquid silicate composition with the bulk mantle composition that is predicted from the proposed models, and ultimately to test the hypothesis of the building block of the Earth has similar composition as enstatitechondrite. Experiments at 12GPa and different temperatures were carried with Kawai-type multi-anvil devices at GRC, Ehime University. With increasing temperature from 1500 to 1900°C, the residual crystalline phase assemblage changes from opx+garnet+olivine, garnet+olivine, and to olivine. The melting temperature of Sahara 97072 meteorite at 12 GPa is almost the same as the reported melting relation of Allende meteorite[5]. Olivine is the liquidus phase for Sahara 97072 meteorite at 12 GPa; silicate solidus is about 1700°C and silicate liquidus is 1900°C, wheresilicate liquid coexisting with metallic liquid. At temperature higher than 1800°C, olivine started to melt to periclase + liquid phase. Magnesiowüstitewas detected at the reaction zone between metallic liquid and silicate liquid, which could be caused by the losing of sulfur from sulfide liquid. Ni and Co content in the melt metallic phases increase with temperature. Solidification of metallic phase shows exsolution of a more nickel rich and iron poor metallic phase coexisting with iron-nickel sulfide. The losing of S from metallic liquid phase to either silicate liquid or to the air will cause large changes on the partitioning of siderophile elements between the metallic phases and the silicate phases.

<sup>&</sup>lt;u>References</u>:[1] Javoy, M. (1995): *GRL*, **22**, 2219-2222; [2] Javoy, M. et al. (2010): *Earth and Planetary Science Letters*, **293**, 259-268; [3] Fitoussi, C. and Bourdon, B. (2012): *Science*,**335**, 1477-1480; [4] Lehner, S.W. et al. (2011): *Lunar and Planetary Science Conference*, **42**, 1430; [5] Agee, CB et al. (1995): *Journal of Geophysical Research: Solid Earth*, **100**, 17725-17740.

#### Effective Temperature Condition in the Separation Process of the Core and Mantle

H. Ichikawa<sup>1,2</sup>, J. Hernlund<sup>2</sup>, S. Labrosse<sup>3</sup>, M. Kameyama<sup>1</sup>

<sup>1</sup>Geodynamics research Center, Ehime University <sup>2</sup>Earth-Life Science Institute, Tokyo Institute of Technology <sup>3</sup>Ecole normale supérieure de Lyon Corresponding author's email address: h-ichikawa@sci.ehime-u.ac.jp

It has been long known that the formation of the core transforms gravitational energy into heat and is able to heat up the whole Earth by about 2000 K. However, the distribution of this energy within the Earth is still debated and depends on the core formation process considered. Iron rain in the surface magma ocean is supposed to be the first mechanism of separation for large planets, iron then coalesces to form a pond at the base of the magma ocean. In this process, equilibrium between metal and silicate is achieved within several seconds [1].

Experimental studies of metal-silicate partition coefficient show that pressure-temperature conditions for metal-silicate equilibrium are far beyond the liquidus or solidus temperature for several hundred kelvin [e.g. 2]. However, because equilibration was considered to occur in at the surface of metal pond at the silicate solidus, such high temperature equilibration was rejected as implausible. Instead, lower temperature equilibration with variable oxygen fugacity was proposed as an alternative, although the plausibility of the physical mechanisms invoked in this scenario is also questionable.

In this study, we model iron rain and heating of the magma by viscous dissipation to calculate the effective pressure-temperature conditions for partitioning in this scenario based on parameterizations derived from direct numerical simulation results of cm-scale emulsion of liquid iron in liquid silicates. We have found effective temperature is much higher than the melting temperature of silicate due to the release of gravitational potential energy. We have also found that the magma ocean depth of 1500-2500 km is consistent with estimated compositions of the core and the mantle.

<u>References</u>. [1] Ichikawa, H., Labrosse, S., Kurita, K. (2010): *JGR*, **115**, B01404, doi:10.1029/2009JB006427; [2] Wade, J. & Wood, B. (2005): *EPSL*, **236**, 78-95.

#### Effect of a Stratified Basal Magma Ocean on the Geodynamo

M. Laneuville<sup>1</sup>, J. Hernlund<sup>1</sup>, S. Labrosse<sup>2</sup>, N. Guttenberg<sup>1</sup>

<sup>1</sup>Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo, Japan <sup>2</sup>Département des Sciences de la Terre, Ecole Normale Supérieure, Lyon, France Corresponding author's email address: mlaneuville@elsi.jp

Earth's magnetic field is thought to be sustained by dynamo action in a convecting metallic outer core since at least 3.45 Ga [1]. Convection induces an isentropic temperature gradient that drains  $13\pm3$  TW of heat from the core by thermal conduction [2-4], and suggests that Earth's core has cooled by 1,000 K or more since Earth's formation [4,5]. However, models of Earth's initial thermal evolution following a giant-impact predict rapid cooling to the mantle melting temperature (e.g., [6]).

In order to understand how the core could have retained enough heat to explain the age of the geodynamo, we relax a key assumption of the basal magma ocean model of [7] to allow for the possibility that the magma is stably stratified. Recent giant impact simulations suggest extensive core-mantle mixing [8], which could have produced such a large stratified magma layer at the core-mantle boundary. Turbulent metal-silicate mixing in a magma ocean could also lead to a stable straffication [9].

In the presence of a stable density gradient, heat transfer through the basal magma ocean occurs through conduction and therefore delays heat loss from the core. Partitioning of iron in the liquid phase upon crystallization changes the density profile and triggers convection in the upper part of the basal magma ocean. Our hypothesis suggests that early core cooling is dominated by the timescale on which the stratification is eroded, and a more efficient core cooling (i.e, the amount of heat extracted from the core is closer to what is actually recquired to drive the geodynamo).

<sup>&</sup>lt;u>References</u>. [1] Tarduno, J. et al. (2010): *Science*, **327**, 1238-1240;[2] de Koker, N. et al. (2012): *Proc. Natl. Acad. Sci*, **190**, 4070-4073; [3] Pozzo, M. et al. (2012): *Nature*, **485**, 355-358; [4] Gomi, H. et al. (2013): *Phys. Earth Planet. Inter*, **224**, 88-103; [5] Labrosse, S. (2015): *Phys. Earth Planet.Inter*, in press; [6] Solomatov, V.S. (2007): In *Treatise on Geophysics*, **9**, 91-120; [7] Labrosse, S. et al. (2007): *Nature*, **450**, 866–869; [8] Saitoh, T. and Makino, J. (2013): *Astrophys. J*, **768**, 44; [9] Deguen et al. (2011): *Earth Planet. Sci. Lett*, **310**, 303-313.

## Major Element Composition of the Early Enriched Reservoir: Constraints from <sup>142</sup>Nd/<sup>144</sup>Nd Isotope Systematics in the Early Earth and High-pressure Melting Experiments of Primitive Peridotite

N. Kondo<sup>1</sup>, T. Yoshino<sup>2</sup>, K.N. Matsukage<sup>3</sup>, T. Kogiso<sup>4</sup>

<sup>1</sup>Gradudate School of Human and Environmental Studies, Kyoto University <sup>2</sup>Institute for Study of the Earth's Interior, Okayama University <sup>3</sup>Tokyo Institute of Technology Corresponding author's email address: kondo.nozomi.75x@st.kyoto-u.ac.jp

Present Accessible Silicate Earth (ASE) has significantly higher <sup>142</sup>Nd/<sup>144</sup>Nd than chondrites [1]. In order to compensate the difference between ASE and chondrites, there should have been low <sup>142</sup>Nd/<sup>144</sup>Nd reservoir, which formed as melt in the early Earth (Early Enriched Reservoir, EER). The major element composition of EER has been still unclear, though it is crucial to estimate its chemical and physical properties, and essential to understand the origin and destiny of EER, which affects present composition of the Earth. In order to determine the major element composition of EER, on the basis of the Sm-Nd partitioning and its dependence on pressure, temperature, and melting phase relation. We determined the major element composition of EER at the estimated pressure-temperature condition, with high-pressure melting experiments of the primitive peridotite, and calculated density of EER.

The EER was estimated to have formed within 33.5 Myr after the solar system formation and at near-solidus temperature at a shallow upper mantle pressure. The result of our experiments and previous studies indicate that the near-solidus melt is Fe-komatiitic at 7 GPa, and picritic to basaltic at pressure less than 3 GPa. The estimated density of the near-solidus melt is smaller than that of the primitive peridotite, suggesting that EER ascended in the mantle, and formed crust. Because the mantle potential temperature would have been very high in the Hadean, EER should have formed at high pressure, and therefore its composition would have been Fe-rich komatiitic to picritic. Because the EER formation precedes to the Moon forming last giant impact, EER, the Hadean komatiitic-picritic crust, was probably spattered from the Earth before or at the last giant impact. Thus EER has been lost, leaving the present Earth non-chondritic.

References. [1] Boyet, M & Carlson, R. W. (2005): Science, 309, 576-581.

#### Ab initio Electrical Resistivity of hcp Iron at Earth's inner Core Conditions

## H. Dekura

## Geodynamics Research Center, Ehime University Corresponding author's email address: dekura.haruhiko.mf@ehime-u.ac.jp

Electrical resistivity of minerals at high-pressure and temperature is one of the most unconstrained properties in deep Earth science. Determination of the electrical resistivity of iron, as a major component of the Earth's core, is essential to discuss its dynamics. Direct experimental determination is known extremely difficult. On the other hand, recent development in computational physics is now accessible to calculations of the electron transport property at even multi-megabar and thousands Kelvin. We have been developing a technique to compute electron-phonon interaction and electrical resistivity of minerals based on the density-functional perturbation theory with the Bolthzmann electron transport theory. In this presentation, I will show the detailed information of the method and show a preliminary result of resistivity of hcp Fe calculated at the conditions corresponding to center of the Earth.

## Hugoniot and Temperature Measurements of H<sub>2</sub>O up to 260 GPa Under Laser-driven Shock Loading

<u>T. Kimura</u><sup>1</sup>, N. Ozaki<sup>2,3</sup>, T. Sano<sup>4</sup>, T. Okuchi<sup>5</sup>, T. Sano<sup>2</sup>, K. Shimizu<sup>6</sup>, K. Miyanishi<sup>2</sup>, T. Terai<sup>2</sup>, T. Kakeshita<sup>2</sup>, Y. Sakawa<sup>4</sup>, R. Kodama<sup>2,3</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University <sup>2</sup>Graduate School of Engineering, Osaka University <sup>3</sup>Photon Pioneers Center, Osaka University <sup>4</sup>Institute of Laser Engineering, Osaka University <sup>5</sup>Institute for Study of the Earth's Interior, Okayama University <sup>6</sup>KYOKUGEN Center for Science and Technology under Extreme Conditions, Osaka University Corresponding author's email address: t kimura@sci.ehime-u.ac.jp

Pressure, density, and temperature data for  $H_2O$  were obtained up to 260 GPa by using laser-driven shock compression technique. The diamond cell applied for the laser shock experiments was used as the sample container in order to achieve temperature conditions lower than the principal Hugoniot states. This shock technique combined with the high-pressure cell can be used for an assessment the equation of state models because it is possible to compare the states under the conditions that the contrast between the models clearly appears. Our *P-r-T* data are in totally agreement with those of the model based on quantum molecular dynamics calculations. These facts indicate that this model is adopted as the standard for modeling interior structures of Neptune, Uranus, and exoplanets in the liquid phase in the mult-Mbar range[1].

References. [1] Kimura, T. et al. (2015): J. Chem. Phys., 142, 164504.

#### High-pressure in situ X-ray Laminography Using Diamond Anvil Cell

## <u>R. Nomura<sup>1</sup></u>, K. Uesugi<sup>2</sup>

<sup>1</sup>Earth-Life Science Institute, Tokyo Institute of Technology, <sup>2</sup>JASRI/SPring-8 Corresponding author's email address: nomura.r.ab@m.titech.ac.jp

Diamond anvil cell (DAC) is a powerful tool to reproduce high pressure (P) and high temperature (T) conditions corresponding to the deep Earth interiors in a laboratory [*e.g.* 1]. Various types of measurements such as *in situ* high *P*-*T* spectroscopies and *ex situ* chemical analysis have been conducted using DAC to understand the physics and chemistry of the Earth materials.

Among them, 3D visualization and textural/chemical characterization of the internal structure of the sample at high *P*-*T* is of great importance. *In situ* high-*P* x-ray computed tomography (CT) has been developed by transmitting x-rays through a sample and a light metal gasket (e.g. Be) between diamond anvils. Recently, the dihedral angle of molten iron between bridgmanite was investigated at high-pressure by using laser-heated DAC combining with x-ray computed tomography (CT) with profound implications for the physical process of the Earth's core-mantle separation [2]. On the other hand, Tsuchiyama et al. (2013) [3] developed "chemical imaging" techniques known as analytical dual-energy microtomography in which the two x-ray energies below and above the absorption energy of a targeted element are used for imaging. Although this technique is powerful for chemical purpose, an application to *in situ* high *P-T* remains technically challenging because typical Earth's major elements have an absorption edge in near soft x-ray energy, in which even Be gasket absorbs the incident x-rays crucially.

X-ray laminography, which has an inclined rotational axis to x-ray, is a suitable technique to apply for diamond anvil cell because x-ray can avoid the gasket to obtain projection images. This technique is generally used to obtain the internal structures of a laterally-extended objects in three dimensions. Although x-ray laminography loses the quantitative information of linear attenuation coefficients, it is still useful for qualitative chemical analysis by combining dual energy x-ray techniques.

In this presentation, we will show our recent developments on *in situ*high pressure x-ray laminography techniques by using a diamond anvil cell.

<sup>&</sup>lt;u>References</u>. [1] Tateno, S. et al. (2010): *Science*, **330**, 359-361; [2] Shi, C. (2013): *Nature Geoscience*, **6**, 971-975; [3] Tsuchiyama, A. et al. (2013): *Geochim. Cosmochim. Acta*, **116**, 5-16.

#### Phase Relations of FeH at Earth's Core Pressure

C. Kato<sup>1</sup>, K. Ohta<sup>1</sup>, K. Hirose<sup>2,3</sup>, Y. Ohishi<sup>4</sup>

<sup>1</sup>Department of Earth and Planetary Sciences, Tokyo Tech <sup>2</sup>Earth-Life Science Institute, Tokyo Institute of Technology, <sup>3</sup>JAMSTEC, <sup>4</sup>JASRI Corresponding author's email address: kato.c.ab@m.titech.ac.jp

Hydrogen is one of the plausible candidates of light element(s) in the Earth's core. Previous studies suggested that hydrogen preferentially partitioned into liquid metallic iron core as FeHx in the magma ocean of the primordial Earth. [e.g., 1, 2]. In-situ X-ray diffraction experiments revealed that FeHx with double-hexagonal close packed (dhcp) structure formed at 3.5 GPa and the structure did not change up to at least 80 GPa [3,4]. Energetic calculations indicate the structural transition of dhcp to hexagonal close packed (hcp), and hcp to face-centered cubic (fcc) structure at the Earth's lower mantle pressure [5]. However, the suggested phase transitions of FeHx have not been verified by experiments, and therefore the crystal structure of FeHx under core pressures is still an open question.

We examined the phase relations of FeHx at high pressures and high temperatures in a laser-heated diamond-anvil cell based on synchrotron X-ray diffraction measurements at BL10XU, SPring-8. The results show that dhcp-FeHx disappeared and hcp-FeHx formed at ~60 GPa, and hcp-FeHx underwent transformation into fcc-FeHx at ~70 GPa. We also obtained the pressure-volume (*P-V*) data of fcc-FeHx at 26 to 137 GPa and 300 K. The compressivity showed a discontinuous change at ~70 GPa, which may be induced by a magnetic transition of fcc-FeHx, as indicated by the theoretical calculation [5]. Based on our experimental results, we argue that a likely crystal structure of FeHx at least at the Earth's topmost core conditions is fcc structure rather than dhcp and hcp.

<u>References</u>. [1] Fukai. (1984): *Nature*, **208**, 174-175; [2] Okuchi et al. (1997): *Science*, **278**, 1761-1784; [3] Badding et al. (1991): *Science*, **253**, 421–424. [4] Hirao et al. (2004): *GRL*, **31**, L06616; [5] Isaev et al. (2007): *PNAS*, **104**, 9268-9171.

#### The Eutectic Liquid Composition in the Fe-Fe<sub>3</sub>S Binary System at the Core Pressure Range

<u>Y. Mori</u><sup>1</sup>, S. Tateno<sup>2</sup>, K. Hirose<sup>3</sup>, G. Morard<sup>4</sup>, Y. Ohishi<sup>5</sup>

<sup>1</sup>Department of Earth and Planetary Sciences, Tokyo Institute of Technology <sup>2</sup>Institute for Study of the Earth's Interior, Okayama University <sup>3</sup>Earth-Life Science Institute, Tokyo Institute of Technology <sup>4</sup>IMPMC, Universite Pierre-et-Marie-Curie <sup>5</sup>Japan Synchrotron Radiation Research Institute Corresponding author's email address: mori.y.ah@m.titech.ac.jp

Sulfur is considered to be an important component in the Earth's core because it is depleted in the crust and mantle compared to other volatile elements and often included in iron meteorites. Here we examine the liquidus phase relations in the Fe-Fe<sub>3</sub>S binary system between 38 and 138 GPa based on characterization of a sample recovered from a melting experiment at high pressure and temperature in a laser-heated diamond-anvil cell. Both Fe-8wt.%S and Fe-14wt.%S samples were employed as starting materials, which were homogeneous mixtures of fine-grain Fe and FeS (<1 µm) prepared by induction melting and rapid quenching technique [1]. We used a focused ion beam (FIB) equipped with energy dispersive X-ray spectrometry (EDS) for textural and chemical characterizations of recovered samples. The samples exhibited a melting texture with quenched liquid alloy at the hottest part and solid Fe or Fe<sub>3</sub>S at its outside. In a couple of samples, the guenched liquid was in direct contact with solid Fe<sub>3</sub>S, and solid Fe was also present right next to Fe<sub>3</sub>S, suggesting that the composition of such liquid is close to a eutectic composition (~12 wt.% S at 66 GPa and ~10 wt.% S at 138 GPa). Indeed, this interpretation is consistent with the results of other experiments obtained in this study. Our data demonstrate that the eutectic liquid composition in the Fe-Fe<sub>3</sub>S binary system decreases its sulfur concentration with increasing pressure, which is in agreement with previous studies [2,3]. The sulfur content in the eutectic liquid composition may be less than 10 wt.% at the inner core boundary pressure. The recent shock-wave study by Huang et al. [2013 GRL] suggested 10 wt.% S in the outer core, but the present study indicates that such liquid alloy with 10 wt.% S crystalizes the B2 phase of Fe-S alloy and thus does not support the sulfur-rich outer core.

<u>References</u>. [1] Morard et al. (2011): *PCM*, **38**, 767-776; [2] Morard et al. (2008): *EPSL*, **272**, 620-626; [3] Kamada et al. (2012): *EPSL*, **359**, 26-33.

## Some Thermodynamic Properties of Larnite ( $\beta$ -Ca<sub>2</sub>SiO<sub>4</sub>) Constrained by High *T*/*P* Experiment and/or Theoretical Simulation

Z.H. Xiong<sup>1</sup>, X. Liu<sup>2</sup>, S.R. Shieh<sup>3</sup>,

<sup>1</sup>Geodynamics Research Center, Ehime University <sup>2</sup>School of Earth and Space Science, Peking University <sup>3</sup>Department of Earth Sciences, University of Western Ontario Corresponding author's email address: xiong.zhihua.gf@ehime-u.ac.jp

Natural larnite (Lrn;  $\beta$ -Ca<sub>2</sub>SiO<sub>4</sub>; space group  $P2_1/n$  with Z = 4) was firstly reported in the Larne district of Great Britain [1], and soon documented on the island of Muck in Scotland[2] and the Tokatoka region in New Zealand [3]. It usually locates in the contact zone between an igneous rock like dolerite or andesite, and a calcitic rock such as chalk or limestone [1, 3]. This conventional field occurrence of Lrn was recently supplemented with another completely different appearance, tiny mineral inclusions, usually coexisting with the walstromite-structured CaSiO<sub>3</sub> (Wal) and titanite-structured CaSi<sub>2</sub>O<sub>5</sub> (Ttn), in diamonds possibly originating from the lower mantle [4, 5, 6]. This new appearance strongly argues that some portions of the deep interior of the Earth are significantly Ca-richer than the normal pyrolitic mantle [7].

In study, pure larnite ( $\beta$ -Ca<sub>2</sub>SiO<sub>4</sub>; Lrn) was synthesized at 6 GPa and 1473 K for 6 hours by using a cubic press, its thermal expansivity was investigated up to 923K by using an X-ray powder diffraction technique (ambient P), and its compressibility was investigated up to  $\sim 16$ GPa by using a diamond-anvil cell coupled with synchrotron X-ray radiation (ambient T). Its volumetric thermal expansion coefficient ( $\alpha_V$ ) and isothermal bulk modulus ( $K_T$ ) were constrained as  $\alpha_V = 4.24(4) \times 10^{-5}$ /K and  $K_T = 103(2)$  GPa (the first pressure derivative  $K_T$ obtained as 5.4(4)), respectively. Its compressibility was further studied with the CASTEP code using density functional theory and planewave pseudopotential technique. We obtained the  $K_T$ values as 123(3) GPa (LDA; high boundary) and 92(2) GPa (GGA; low boundary), with the values of the  $K_T$  as 4.4(9) and 4.9(5), respectively. The phonon dispersions and vibrational density of states (VDoS) of Lrn were simulated using density functional perturbation theory, and the VDoS was combined with a quasi-harmonic approximation to compute the isobaric heat capacity ( $C_P$ ) and vibrational entropy ( $S_{298}^0$ ), yielding  $C_P = 212.1(1) - 9.69(5) \times 10^2 T^{0.5}$  –  $4.1(3) \times 10^{6} T^{2} + 5.20(7) \times 10^{8} T^{3}$  J mol<sup>-1</sup> K<sup>-1</sup> for the T range of ~298-1000 K and  $S_{298}^{0} = 129.8(13)$ J mol<sup>-1</sup> K<sup>-1</sup>. In addition, the microscopic and macroscopic thermal Grüneisen parameters of Lrn at 298 K were calculated to be 0.75(6) and 1.80(4), respectively.

References. [1] Tilley, C.E. (1929): Mineral Mag, 22, 77-86; [2] Tilley, C.E. (1947): B Com Geol Finlande, 140, 97-106; [3] Mason, B. (1957): Am Mineral, 42, 379-392; [4] Joswig, W., Stachel, T.H., Harris, J.W., Baur, W.H. and Brey, G.P. (1999): Earth Planetary Sci Lett, 173, 1-6; [5] Nasdala, L., Brenker, F.E., Glinnemann, J., Hofmeister, W., Gasparik, T., Harris, J.W., Stachel, T. and Reese, I. (2003): Eur J Mineral, 15, 931-935; [6] Brenker, F.E., Vincze, L., Vekemans, B., Nasdala, L., Stachel, T., Vollmer, C., Kersten, M., Somogyi, A., Adams, F., Joswig, W. and Harris, J.W. (2005): Earth Planetary Sci Lett, 236, 579-587; [7] Ringwood, A.E. (1975): McGraw-Hill, New York.

#### The Lower Mantle: A Seismological Perspective

#### B.L.N. Kennett

## Research School of Earth Sciences, The Australian National University Corresponding author's email address: Brian.Kennett@anu.edu.au

The structure of the lower mantle appeared to be simple when summarized by 1-D earth models, but has become progressively more complex as we have learnt more about the 3-D structure of the Earth. The point at which one leaves the mantle transition zone and enters the lower mantle is not well defined, but can be conveniently taken as the depth at which majorite garnet is extinguished (around 850 km deep) where viscosity reaches a high value. Away from the major sources of colder material in former subduction zones, the levels of seismic heterogeneity are modest though stronger in shear wavespeed than bulk-sound speed. Such heterogeneity increases significantly below 2100 km depth, though this is not what is expected from the effect of pressure. The increase in wavespeed variability occurs well before any influence from post-perovskite material could be expected.

Different styles of investigation give very consistent pictures of the major features in lower mantle structure and support the presence of zones of lower wavespeed material rising well into the middle mantle. It is tempting to regard wavespeed reduction as due to temperature, but the relative behavior of the bulk and shear moduli suggests that chemical heterogeneity cannot be ignored. Recent work using full-waveform inversion of long-period seismograms suggests that some lower wavespeed material may be organized into relatively narrow features beneath recognized hot spots - are these the elusive plumes?

#### Persistence of Strong Silica-Enriched Domains in the Earth's Lower Mantle

<u>J.W. Hernlund<sup>1</sup></u>, C. Houser<sup>1</sup>, M.D. Ballmer<sup>1,2</sup>, R. Wentzcovitch<sup>1,3</sup>, K. Hirose<sup>1</sup>

<sup>1</sup>Earth-Life Science Institute, Tokyo Institute of Technology, Meguro, Tokyo, Japan <sup>2</sup>Institute of Geophysics, ETH Zurich, Zurich, Switzerland <sup>3</sup>Chemical Engineering and Materials Science Department, University of Minnesota

The chemical composition of the Earth's lower mantle, the largest region of our planet, ispoorly constrained. While some geochemical observations suggest a lower mantle bulk com-position that differs from the shallow mantle, geophysical evidence suggests that whole mantle convection and associated mixing should have largely erased any major differences. Herewe use numerical models of mantle convection to show that large silica-enriched domains in the lower mantle are stable against mixing owing to a modest increase in density and higherviscosity that results from greater abundance of the strong (Mg,Fe)SiO3-bridgmanite mineral phase. The style of mantle convection in such circumstances exhibits strong cores ofbridgmanite enriched ancient mantle structures (BEAMS) separated by conduits of weakersilica-depleted rocks that circulate between the shallow and deep mantle. This pattern of convection is stable over timescales much longer than the age of the Earth, even for relativelymodest viscosity and density increases in BEAMS material, thus permitting significant com-position differences between the deeper and shallower mantle to be compatible with whole 1 mantle convection. Our models exhibit strong memory effects upon lower mantle convectiveplanform, stabilizing the location of upwelling and downwelling flows through the deep man-tle over billions of years. The BEAMS model may help to reconcile differences between the composition of the shallow mantle and that of the Sun and chondritic meteorites.

## Discovery of New Iron Oxide Fe<sub>7</sub>O<sub>9</sub> and Its Solid Solution, (Mg,Fe<sup>2+</sup>)<sub>3</sub>Fe<sup>3+</sup><sub>4</sub>O<sub>9</sub>

<u>R. Sinmyo</u><sup>1,\*</sup>, E. Bykova<sup>1</sup>, SV. Ovsyannikov<sup>1</sup>, C. McCammon<sup>1</sup>, I. Kupenko<sup>2</sup>, L. Ismailova<sup>1</sup>, L. Dubrovinsky<sup>1</sup>

<sup>1</sup>Bayerisches Geoinstitut, Universitaet Bayreuth <sup>2</sup>Europian Synchrotron Radiation Facility, \*Now at Earth-Life Science Institute Tokyo Institute of Technology Corresponding author's email address: ryosuke.sinmyo@elsi.jp

Iron oxides are fundamentally important compounds for the terrestrial planets. The stability and properties of iron oxides are essential information to understand the evolution of redox state of the Earth's mantle and surface. Here we report new high-pressure polymorphs of iron oxide  $Fe_7O_9$  ( $Fe^{3+}/Fe^{2+} = 4/3$ ) and its  $Fe^{2+}$ -Mg solid solution (Mg, $Fe^{2+}$ )<sub>3</sub> $Fe^{3+}_4O_9$  that can be recovered at ambient conditions. We synthesized single crystals of the both compounds at about 24-26 GPa using a multi-anvil press. Single crystal X-ray diffraction (XRD) studies showed that the crystal structures of both  $Fe_7O_9$  and (Mg, $Fe^{2+}$ )<sub>3</sub> $Fe^{3+}_4O_9$  have monoclinic *C2/m* space groups, that differ from any other known lattices of iron oxides. Mössbauer spectra are in agreement with the crystal structure refined from single crystal XRD. This newly found  $Fe_7O_9$  polymorph suggests that iron oxides may have more variable mixed valence state under high-pressure condition than previously thought. Based on analogy with  $Fe^{2+}_{1+n}Fe^{3+}_2O_{4+n}$  group, a  $Fe^{2+}_{3\pm n}Fe^{3+}_4O_{9\pm n}$  group might be also stable at certain high pressures and temperatures and oxygen fugacity. Some  $Fe^{3+}$ -rich phase found in diamond inclusion may be a back-transformed high-pressure polymorph of these iron oxides. The phase relation of such new iron-oxide group may provide a new insight for redox state of the Earth's mantle.

#### Helium Diffusion in Mantle Minerals from First Principles

#### John Brodholt (UCL)

We have used ab initio DFT methods to calculate the diffusion coefficients of He in olivine, perovskite and post-perovskite under lower mantle conditions. The diffusion coefficients were calculated using the nudged-elastic band method to find the minimum energy pathway and the migration enthalpy. The harmonic Vinyard theory was used to calculate the migration entropy and attempt frequency. In perovskite and post-perovskite, He diffusion is so fast that we can also estimate the diffusion coefficient directly in an ab initio molecular dynamics simulation. The two methods agree well with each other.

The diffusion coefficients of He in olivine agree extremely well with existing experiments and is fast. For instance, in the upper mantle He can diffuse between 1 and 50 meters in 1 million years. Interestingly, diffusion in perovksite is even faster (perhaps by two orders of magnitude) and in the deepest Earth, diffusion coefficients are sufficiently high so as to be able to homogenise reservoirs of up to 50 km over the age of the Earth. The source of high <sup>3/4</sup>He reservoirs must, therefore, be larger than this if they are to exist for the age of the Earth. Moreover, larger reservoirs of high <sup>3/4</sup>He will essentially pollute the mantle around them and potentially some high <sup>3/4</sup>He signals at the surface will be decoupled from other "hotspot"-like isotopic signals.

Finally, our results suggest that He solubility in the lower mantle is much smaller than in the upper mantle. This is supported by some experiments in the multi-anvil we have performed.

#### Modes of Slab Behavior: from the Transition Zone to the Mid-Lower Mantle

## <u>C.R. Bina<sup>1</sup></u>, H. Čížková<sup>2</sup>

<sup>1</sup>Department of Earth and Planetary Sciences, Northwestern University, U.S.A <sup>2</sup>Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic Corresponding author's email address: craig@earth.northwestern.edu

Subducting slabs may exhibit buckling instabilities and consequent folding behavior in the mantle transition zone, accompanied by temporal variations in dip angle, plate velocity, and trench retreat. Governing parameters include both viscous (rheological) and buoyancy (thermo-petrological) forces. Numerical experiments suggest that many parameter sets lead to slab deflection at the base of the transition zone, typically accompanied by quasi-periodic oscillations in largely anticorrelated plate and rollback velocities, resulting in undulating stagnant slabs as buckle folds accumulate subhorizontally atop the lower mantle. Slab petrology – of mantle phase transitions and hydrated crust – is a dominant factor in this process [1]. For terrestrial model parameters, trench retreat is common and trench advance quite rare, due to rheological and ridge-push effects. Global plate-motion studies indicate that trench advance is rare on Earth, too, being largely restricted to the Marianas-Izu-Bonin arc. Dynamical models based on the unusual double-subduction geometry of the Philippine Sea region do yield persistent trench advance [2].

Imaging of buckled stagnant slabs is complicated by smoothing effects inherent in seismic tomography, but velocity structures for petrologically layered slabs, spatially low-pass filtered for comparison with tomography of corresponding resolution, yield a better fit to  $V_P$  anomalies from stagnant slab material beneath northeast China for undulating (vs. flat-lying) slabs [3]. Earthquake hypocentral distributions and focal mechanisms (especially below 660 km) also provide insights into slab buckling in regions of slab stagnation [4], and these can be compared to stress fields computed from our dynamical models.

A combination of driving forces governs slab stagnation. Buoyancy arising from thermal perturbation of equilibrium phase transitions contributes to slab bending and may partly control depth of stagnation [5]. Additional buoyancy from possible metastable persistence of olivine or pyroxene phases may enhance slab stagnation, and temporal decay of such metastability by thermal equilibration may lead to slab foundering [5, 6, 7, 8, 9]. Complexities in mantle viscosity structure, associated with mineralogical transitions, may also contribute to slab stagnation [1, 10].

Subsequent descent of buckled slab material into the lower mantle may occur in a variety of ways: drawn downward from the distal (relative to the trench) edge, from the proximal edge, or from somewhere in between [11], or by bulk foundering of the entire megalith-like mass. Mode selection appears to be governed by factors such as rheological structure and trench motion.

Presence of foundered slab material is likely indicated by seismic scatterers observed in the mid-lower mantle [12]. Proposed origins of such scatterers include: structural transitions in relict silica phases [13], electronic spin transitions in hydrous ferromagnesian silicates [14], and electronic spin transitions in alkalic hexagonal aluminous phases [15], all occurring primarily within subducted crustal material.

<sup>WITHIN SUDDUCTED CRUSTAL MATERIAL.
<u>References</u>. [1] Čížková, H. & Bina, C.R. (2013):</sup> *EPSL*, **379**, 95-103; [2] Čížková, H. & Bina, C.R. (2015): *EPSL*, **430**, 408-415; [3] Zhang, Y. et al. (2013): *GGG*, **14**, 1182-1199; [4] Fukao, Y., et al. (2014): JpGU abst., SIT03-12;
[5] Bina, C.R. & Kawakatsu, H. (2010): *PEPI*, **183**, 330-340; [6] Bina, C.R. (2013): *Nature Geosci*, **6**, 335-336; [7]
Bina, C.R. (2013): IWMMLD abst., 39; [8] Agrusta, R., van Hunen, J., Goes, S. (2014): *GRL*, **41**, 8800-8808; [9]
King, S.J., Frost, D.J., Rubie, D.C. (2015): *Geology*, **43**, 231-234; [10] Marquardt, H. & Miyagi, L. (2015): *Nature Geosci*, **8**, 311-314; [11] Christensen, U.R. (1996): *EPSL*, **140**, 27-39; [12] Kaneshima, S. & Helffrich, G. (2010): *PEPI*, **183**, 91-103; [13] Bina, C.R. (2010): *PEPI*, **183**, 110-114; [14] Chang, Y.-Y. et al. (2013): *EPSL*, **382**, 1-9; [15] Wu, Y. et al. (2014): AGU abst., MR24-04.

#### **Multiscale Seismic Tomography and Mantle Dynamics**

#### D.P. Zhao

## Department of Geophysics, Tohoku University, Sendai, Japan Corresponding author's email address: zhao@aob.gp.tohoku.ac.jp

We determined a new global P-wave tomography model using a flexible-grid parameteri-zation, 3-D ray tracing and five kinds of mantle phases (P, pP, PP, PcP & Pdiff) [1, 2]. This new model better reveals the mantle structure under the polar regions than the previous models. The subducting slabs are generally imaged clearly as high-velocity (high-V) zones. The young slabs are still subducting in the upper mantle and the mantle transition zone (MTZ), whereas the old and ancient slabs are either stagnant in the MTZ or have subducted down to the lower mantle, even reaching the core-mantle boundary. Low-velocity (low-V) anomalies are generally revealed in the mantle under the hotspot regions. It seems that a variety of mantle upwelling (plumes) exist. Some strong plumes are visible in the whole mantle under the long-living hotspots, whereas weak plumes are visible in only some depth range under the minor hotspots. Beneath the intraplate volcanoes in East Asia, Bering Sea and West Alaska, significant low-V anomalies are revealed in the upper mantle, which may reflect hot and wet upwelling associated with corner flows in the <u>Big Mantle Wedge (BMW)</u> above the stagnant Pacific slab in the MTZ and perhaps deep slab dehydration as well. The subduction-triggered magmatism in the BMW may be a new class of mantle plumes.

Our high-resolution regional tomography revealed more details on the origin of the intraplate volcanism in East Asia [2-4]. The active Tengchong volcano in Southwest China is underlain by a prominent low-V anomaly in the shallow mantle, which may be caused by the subduction and dehydration of the Burma microplate plate (or the Indian plate). The Hainan volcano is underlain by a plume-like low-V anomaly that extends down to at least 1000 km depth and seems to be related to the deep subductions of the Burma microplate (or the Indian plate) in the west and the Philippine Sea plate in the east. Prominent low-V anomalies are detected beneath the Changbai, Longgang and Xianjindao volcanoes in Northeast Asia, which may be related to the rollback of the subducting Pacific slab as well as convective circulation processes in the BMW above the stagnant slab. The origin of the Wudalianchi volcano in Northeast China seems associated with the upwelling of asthenospheric materials caused by subduction-induced lithospheric delamination.

We also determined P-wave anisotropic tomography of the Western Pacific subduction zones and SE Asia [4, 5]. The P-wave azimuthal anisotropy exghibits a fast-velocity direction (FVD) of NE-SW (trench parallel) in the subducting Philippine Sea slab beneath the Ryukyu arc, which is consistent with the spreading direction of the West Philippine Basin during its initial opening stage, suggesting that it may reflect a fossil anisotropy. A striking variation of the FVD with depth is revealed in the subducting Pacific slab beneath the Northeast Japan 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 Northeast Japan and Ryukyu arcs is trench normal, which reflects subduction-induced convection. Beneath the Kuril and Izu-Bonin arcs where oblique subduction occurs, 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 there.

<u>References</u>. [1] Zhao, D. et al. (2013): Gondwana Res, 23, 595-616; [2] Zhao, D. (2015): Multiscale Seismic Tomography. Springer, 304; [3] Wei, W. et al. (2012): J. Asian Earth Sci, 60, 88-103; [4] Wei, W. et al. (2015): J. Geophys.Res, 120, 1642-1666; [5] Huang, Z. et al. (2015): J. Geophys.Res, 120, 5154-5174.

## Three-dimensional Analysis of Pore Effect on Composite Elasticity by Means of Finite Element Method

#### A. Yoneda

#### ISEI, OkayamaUniversity

A three-dimensional buffer-layer finite element method (FEM) model was developed to investigate the porosity effect on macroscopic elasticity. Using the three-dimensional model, the effect of pores on bulkeffective elastic properties were systematically analyzed by changing the degree of porosity, the aspect ratio of the ellipsoidal pore, and the elasticity of the material. The present results in 3D space were compared with the previous ones in 2D space. Derivatives of normalized elastic stiffness constants with respect to needle-type porosity are integers, if the Poisson ratio of a matrix material is zero; those derivatives of normalized stiffness elastic constants for  $C_{33}$ ,  $C_{44}$ ,  $C_{11}$ , and  $C_{66}$  converge to -1, -2, -3, and -4, respectively, at the corresponding condition. We proposed a criterion of R < 1/3, where the mutual interaction between pores becomes negligible for macroscopic composite elasticity. These derivatives are nearly constant below 5% porosity in the case of spherical pore, suggesting that the interaction between neighboring pores is insignificant if the representative size of the pore is less than one-third of the mean distance between neighboring pores. The relations we obtained in this work were successfully applied to invert bulk modulus and rigidity of Cmcm-CaIrO<sub>3</sub> as a case study: the performance of the inverting scheme was confirmed through this assessment. Thus the present scheme is applicable to predict macroscopic elasticity of porous object as well.

#### Semi Analytical Model for the Effective Grain Size Profile in the Mantle of the Earth

<u>A. Rozel<sup>1</sup></u>, G. Golabek<sup>2</sup>, M. Thielmann<sup>2</sup>, P.J. Tackley<sup>1</sup>

<sup>1</sup>ETH Zurich, <sup>2</sup>Bayreurisches Geoinstitut Corresponding author's email address: antoinerozel@gmail.com

We present a semi analytical model of mantle convection able to predict the grain size profile of the present day Earth. Grain size evolution has been studied with increasing interest over the last decades but its behavior in both mantle and lithosphere remains largely misunderstood due to its non-linearity. Several recent studies suggest that it might play a fundamental role in localization of deformation in the lithosphere but we focus here on the mantle in which we also observe important processes.

We propose a 1D compressible thermal convection model based on the equality of advective heat flux and the integral of viscous dissipation in the whole domain. Imposing mass conservation, our model is able to predict all rheological parameters able to produce both present day average surface velocity and lower mantle viscosity. Composite rheologies involving dislocation creep and grain size dependent diffusion creep are considered. The effect of phase transitions on the grain size is also explicitly taken into account. We present the family of solutions for the activation volume and the viscosity jump at the 660 discontinuity according to any initial choice of activation energy. The scaling laws for rheological parameters obtained are compared to self-consistent evolutionary simulations of mantle convection considering grain size dependent diffusion creep in 2D spherical annulus geometry.

## The Relationship of Crystallographic Orientation between Perovskite and Post-Perovskite During Phase Transformation

D. Yamazaki<sup>1</sup>, M. Murakami<sup>2</sup>, F. Xu<sup>1</sup>, N. Hirao<sup>3</sup>, Y. Seto<sup>4</sup>

<sup>1</sup>ISEI, Okayama University, <sup>2</sup>Graduate school of Science, Tohuku University <sup>3</sup>Japan Synchrotron Radiation Research Institute <sup>4</sup>Kobe University Corresponding author's email address: dy@misasa.okayama-u.ac.jp

In the D" layer of the earth's lower mantle is characterized by the seismic anomalies, for example, velocity discontinuity, anisotropy and lateral heterogeneity [e.g., 1]. The dominant phase in the D" layer is considered to be post-perovskite of (Mg,Fe)SiO<sub>3</sub> and hence their mineralogical properties are essential to understand the dynamics of the lower mantle. The observed seismic anisotropy can be explained by the lattice preferred orientation of the constituent materials [2]. One possible mechanism to form the lattice preferred orientation of post-perovskite is topotactic relation between perovskite grain and post-perovskite grain during phase transformation because the lattice preferred orientation of perovskite is likely formed due to deformation during slab subduction. In this study, we investigated the topotactic relation by means of high pressure experiments in (Mg, Fe)SiO<sub>3</sub> by using a diamond anvil cell and in CaIrO<sub>3</sub> as an analogue by using piston cylinder apparatus.

In the series of experiments on CaIrO<sub>3</sub>, the coarse-grained polycrystalline perovskite was firstly prepared as starting material. Then, at 1 GPa, the starting materials were partially transformed into perovskite. After experiments, the crystallographic orientation was determined on the polished surface of the recovered sample by using electron back-scattered diffraction technique. In the experiment on (Mg, Fe)SiO<sub>3</sub>, single crystal of perovskite was compressed to the stability field of post-perovskite (>120 GPa), and it was partially transformed to post-perovskite as well as experiments on CaIrO<sub>3</sub>. In situ determination of crystallographic orientation was performed by using synchrotron X-ray at SPring-8.

In the both series of experiments, we found the topotactic relation between the relict of perovskite and the newly formed post-perovskite grain with *a*-axis of perovskite to *b*-axis of post-perovskite, *b*-axis of perovskite to *a*-axis of post-perovskite and *c*-axis of perovskite to *c*-axis of post-perovskite (Fig. 1). The present results suggest that the lattice preferred orientation of post-perovskite is developed immediately after transformation from perovskite due to the topotactic transition and then the pattern of lattice preferred orientation may be modified by the subsequent deformation of post-perovskite in the D" layer.



Fig.1. Pole figure plots of CaIrO<sub>3</sub> post-perovskite to perovskite.

References. [1] Panning and Romanowicz, (2004): Science, 303, 351; [2] Iitaka et al., (2004): Nature, 430, 442.

#### **Temperature of the Lower Mantle**

<u>C. Houser<sup>1</sup></u>, J. Hernlund<sup>1</sup>, R. Wentzcovitch<sup>2</sup>, J. Valencia-Cardona<sup>2</sup>

<sup>1</sup>Earth-Life Science Institute, Tokyo Institute of Technology <sup>2</sup>University of Minnesota Corresponding author's email address: chouser@elsi.jp

The temperature is as much of an unknown as composition when considering the properties of the lower mantle. The temperature at the base of the mantle transition zone is constrained within 100-200 K by interpreting depths of the 410 and 660 km seismic discontinuities as phase transitions in a mantle with close to a pyrolite composition. The temperature at the core-mantle boundary is constrained by observations of the post-perovskite phase transition and the melting point of a pyrolite or perovskite composition. Pyrolite is the theoretical parent rock that can partially melt to produce basaltic oceanic crust and a harzburgite oceanic lithosphere. Since oceanic lithosphere has been subducted and mixed in the Earth's mantle for billions of years, it is reasonable to assume that the lower mantle could contain an abundance of material with close to a pyrolite composition. However, the Earth's upper mantle appears depleted in Si relative to the sun and most chondrite meteorites, so it may be that the lower mantle is more Si rich than the upper mantle. Since direct experimental measurements of rock velocity and density at actual lower mantle temperatures and pressures are difficult, we currently rely on calculations of velocity and density to explore compositions/geotherms to test their compatibility with seismology and geodynamics. Since the community has not reached a consensus regarding which technique is correct, here I present a variety of temperature profiles of the lower mantle based on Density Function Theory as well as equation of state extrapolations using finite strain At low temperature, these methods are in generally good agreement, but differences theory. emerge above 2000 K, which constitutes most of the lower mantle. Since global seismic observations can constrain the average seismic properties of the lower mantle, it has become common practice to try to fit a computed velocity/density profile to a seismic model, such as PREM, to examine whether or not a proposed composition could represent the dominant mineralogy of the lower mantle. Results depend on the temperature profile which is often set by defining the temperature at the top of the lower mantle and assuming the system is adiabatic as pressure increases. The different methods agree that velocity and density increase as the relative amount of perovskite, or rather bridgmanite, increases, ie. Mg/Si ratio decreases. PREM velocities are slower than pure perovskite and higher than ferropericlase, so some mixture of the two is needed to match the global seismic average. In the past, mixtures with a composition close to pyrolite have been able to fit PREM with reasonable geotherms, but more Si enriched compositions required high temperatures to fit PREM. However, new calculations and experiments suggest that the shear modulus may be lower than previously thought in the lower mantle. In this case, the lower mantle could be more Si enriched or contain regions of Si enrichment for more modest increases in temperature.

#### Waveform Inversion for 3D Structure in D"

## <u>K. Kawai</u>

Department of Earth Science and Astronomy Graduate School of Arts and Sciences, University of Tokyo Corresponding author's email address: kenji@ea.c.u-tokyo.ac.jp

We formulate the inverse problem of waveform inversion for localized 3-D seismic structure, computing partial derivatives of waveforms with respect to the elastic moduli at arbitrary points in space for anisotropic and anelastic media. In this study we minimize computational requirements by using the Born approximation with respect to a laterally homogeneous model, but this is not an inherent limitation of our approach. We solve the inverse problem using the conjugate gradient (CG) method, using Akaike's Information Criterion (AIC) to truncate the CG expansion. We apply our method to invert for 3-D shear wave structure in the lowermost mantle beneath Central America and the western Pacific at periods from 12.5 to 200 s for deep and intermediate-depth events. The resulting model beneath Central America shows lateral heterogeneity in the E-W direction, which may be associated with a subducted cold slab surrounded by hotter materials with slower velocities [1]. We also find two low-velocity zones at the bottom of the target region, with a high-velocity zone in the middle, and a low-velocity zone above the high- velocity zone and contiguous with the two deeper low-velocity zones at a depth of 200-300 km above the core-mantle boundary (CMB) beneath the western Pacific. This supports the idea that the Pacific LLSVP may be an aggregation of small upwelling plumes rather than a single large thermochemical pile [2]. Various tests show that our model is robust.

<u>References</u>. [1] Kawai, K. et al. (2014): *Geophys. J. Int.*, **197**, 495–524; [2] Konishi, K. et al. (2014): *Geophys. J. Int.*, **199**, 1245–1267

## Adjacent High- and Low-Velocity Regions around the Western Edge of the Pacific Large-Low Shear Velocity Province

#### S. Tanaka

#### D-EARTH, JAMSTEC

## Corresponding author's email address: stan@jamstec.go.jp

The Large-Low Shear Velocity Provinces (LLSVPs) beneath Pacific and Africa are widely recognized by global tomographic studies, which characterize the large-scale lateral heterogeneity in the lowermost mantle as well as high-velocity anomalies surrounding the Pacific Ocean [1-3]. The detailed seismic wave analyses have suggested the existence of a sharp boundary of the LLSVPs [4, 5]. Especially, high velocity anomalies are fond to be adjacent to low velocity anomalies near the western edge of the Pacific LLSVP for S-wave below New Guinea [6] and P-wave below Micronesia [7]. Most recent study supports the similar S-wave structure below Micronesia [8].

These results suggest that the material of subducted slabs is not easily assimilated into the surrounding mantle, sometime deeply intruded in the LLSVP. This view is consistent with a mantle dynamics simulation [9], which is based on a hypothesis that the dynamics of the subducted slabs would affect the nature of the LLSVP and distribution of the ultra-low velocity zones (ULVZ).

To confirm this hypothesis, further seismic data collection and analysis will be required. We have a new project of a seismic observation, which aims to contribute to further understanding of the structure and dynamics in such a complicated region.

<sup>&</sup>lt;u>References</u>. [1] Ritsema, J. et al. (2010): *Geophys J Int*, **184**, 1223-1236; [2] Lekic, V. et al. (2012): *Earth Planet Sci Lett*, **357-358**, 68-77; [3] French, S. and Romanowicz, B. (2015): *Nature*, **525**, 95-99; [4] Rirsema, J. et al. (1998): *Geophys Res Let*, **25**, 4245-4248; [5] To, A. et al. (2005): *Earth Planet Sci Lett*, **233**, 137-153; [6] Idehara, K., et al. (2012): *Geophys J Int*, **192**, 1-6; [7] Tanaka, S. et al. (2015): *Geophys J Int*, **200**, 1052-1065; [8] Tanaka, S. and Kawakatsu, H. (2015): JpGU 2015 meeting abstract; [9] McNamara, A. et al. (2010): *Earth Planet Sci Lett*, **299**, 1-9.

#### **Technical Developments on Acoustic Emissions Monitoring at High Pressures**

T. Ohuchi<sup>1</sup>, X. Lei<sup>2</sup>, Y. Higo<sup>3</sup>, Y. Tange<sup>3</sup>, T. Irifune<sup>1,4</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University <sup>2</sup>Institute of Geology and Geoinformation National Institute of Advanced Industrial Science and Technology <sup>3</sup>Japan Synchrotron Radiation Institute <sup>4</sup>Earth-Life Science Institute, Tokyo Institute of Technology Corresponding author's email address: ohuchi@sci.ehime-u.ac.jp

The subduction zone produces a major fraction of the Earth's seismic activity. Intermediate-depth earthquakes within the subducting slab form a double seismic zone. The cause of intraslab seismicity have been attributed to dehydration of hydrous minerals. At deeper depths, dehydration embrittlement (i.e., hydrofracturing) is expected to play an important role in failure of rocks because the overall volume change of the dehydration reaction is positive and thus pore pressure can be increased [1]. However, experimental results on dehydration embrittlement of antigorite are controversial. Dobson et al. [2] conducted a series of experiments on dehydration of antigorite, and they reported that dehydration of antigorite associates acoustic emission (AE) when the dehydration reaction is positive. Recently, Gasc et al. [3] reported that no detectable AEs through dehydration of antigorite-rich serpentinite. Therefore, the cause of intermediate-depth earthquakes is still unclear. In some of subduction zones, a significant activity of deep-focus earthquakes has been reported [4]. It has been proposed that deep-focus earthquakes are triggered by an instability faulting caused by olivine phase transformations [5]. Schubnel et al. [6] conducted deformation experiments on germanium olivine (Mg<sub>2</sub>GeO<sub>4</sub>) at 2-5 GPa and 1000-1250 K, and they observed many AEs generated in the sample. Schubnel et al. [6] discussed that fractures nucleated at the onset of the olivine-to-spinel transition.

To investigate the brittle properties of rocks, determination of AE source is critical. In the community of high-pressure rock physics, Green & Burnley [7] conducted AE monitoring by using a Griggs apparatus combined with an AE sensor. Dobson et al. [8] adopted 4 AE sensors to a multianvil apparatus. However, the position of AE source has not been determined in the experiments because of not enough number of sensors used in the experiments. De Ronde et al. [9] adopted 8 AE sensors to a multianvil apparatus and they succeeded to determine the position of AE sources. Recently, Gasc et al. [3] succeeded to develop an experimental setup that allows determining the position of AE source by using DIA-type multianvil apparatus combined with 6 AE sensors. Schubnel et al. [6] adopted the experimental setup reported by Gasc et al. [3] to a D-DIA apparatus installed at a synchrotron facility, and they succeeded to measure strain and stress of the sample and AE signals. We have developed an experimental setup that is optimized for the determination of the position of AE source in a synchrotron D-DIA apparatus. We will report some preliminary experimental results on AE monitoring under the upper mantle conditions.

<sup>&</sup>lt;u>References</u>. [1] Raleigh, C.B. and Paterson M.S. (1965): *J. Geoophys Res*, **70**, 3965-3985; [2] Dobson, D.P. et al. (2002): *Science*, **298**, 1407-1410; [3] Gasc, J. et al. (2011): *Phys. Earth Planet. Inter*, **189**, 121-133; [4] Kirby, S.H. et al. (1995): *Geophys. Res. Lett*, **22**, 233-2236; [5] Kirby, S.H. et al. (1991): *Science*, **252**, 216-225; [6] Schubnel, A. et al. (2013): *Science*, **341**, 1377-1380; [7] Green, H.W. and Burnley, P.C. (1992): *Nature*, **341**, 733-737; [8] Dobson, D.P. et al. (2004): *Phys. Earth Planet. Inter*, **143-144**, 337-346; [9] De Ronde, A.A. et al. (2007): *Geophys. J. Int*, **171**, 1282-1294.

#### **Creep Behavior of Fe-bearing Olivine under Hydrous Conditions**

M. Tasaka<sup>1,2</sup>, M.E. Zimmerman<sup>2</sup>, D.L. Kohlstedt<sup>2</sup>

<sup>1</sup>Niigata University, <sup>2</sup>University of Minnesota Corresponding author's email address: tasaka@geo.sc.niigata-u.ac.jp

Since iron and hydrogen plays an important role in dynamic processes not only in Earth's mantle but also in Mars's mantle, we conducted uniaxial compression experiments on polycrystalline samples of olivine,  $(Fe_{1-xFo}, Mg_{xFo})_2SiO_4$ , with  $X_{Fo} = 0, 0.53, 0.77, 0.90$ , and 1.0 under hydrous condition. A Paterson-type gas medium apparatus was used for these experiments. The water content determined from Fourier transform infrared (FTIR) spectroscopy analyses of larger Fo<sub>90</sub> crystals embedded in the olivine polycrystalline aggregates demonstrate that the samples are water saturated both before and after deformation. The grain sizes of initial and deformed samples were determined using electron backscatter diffraction (EBSD).

Triaxial-compression tests at 300 MPa confining pressure were conducted at temperatures from 1050 to 1200 °C at constant stress in the range of 25 to 316 MPa. The values of the pre-exponential term, stress and grain size exponents and activation energy in the constitutive equation were determined for a wide range of  $X_{Fo}$ .

At constant temperature, strain rate, and grain size the flow stress of the samples decreases with increasing iron content of olivine. Combining our data with that from Fe-bearing olivine deformed under dry conditions (Zhao et al., 2009 EPSL), we formulated a flow law as a function of X<sub>Fo</sub> under both dry and wet conditions. The overall dependence of the strain rate of olivine on  $X_{Fo}$  is characterized by 2 parameters, directly, through the exponent (m) in the coefficient  $X_{Fo}^{m}$  of the strain-rate and indirectly, through  $\alpha X_{Fo}$  in the activation energy term, such as, (strain rate =  $A^*(stress)^n/(grain size)^{p*}(X_{F0})^m*(water fugacity)^{r*}\exp[-(Q_0+\alpha X_{F0})/RT]$ , where A is creep constant, n is stress exponent, p is grain size exponent, m is iron content exponent, r is water fugacity exponent,  $Q_0$  is activation energy coefficient, a is activation energy coefficient as a function of  $X_{\rm Fo}$ . Assuming an appropriate charge neutrality condition, the experimentally determined value of m is well explained by the silicon vacancy concentration as a function of  $X_{Fo}$ . Similarly, the dependence of the activation energy on  $\alpha X_{Fo}$  can be correlated with a point defect model determined from thermo-gravimetric measurements for Fe-bearing olivine. These features indicate that if we know the charge neutrality condition and point defect model, we are able to reproduce the observed strain rate as a function of X<sub>Fo</sub>, which may be applicable not only to the iron-bearing olivine but also to other solid solution systems.

References. [1] Tasaka, M., M. et al. (2015): J. Geophys. Res. Solid Earth, 120, doi:10.1002/2015JB012096.

#### Stability Region of the (K, Na)AlSi<sub>3</sub>O<sub>8</sub> Hollandite Solid Solution

Y. Zhou<sup>1</sup>, T. Irifune<sup>1,2</sup>, H. Ohfuji<sup>1</sup>, T. Shinmei<sup>1</sup>, W. Du<sup>1,2</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University, Matsuyama 790-8577, Japan <sup>2</sup>Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo 152-8550, Japan Corresponding author's email address: GRC2014917@gmail.com

Aluminosilicate hollandite, with a chemical formula of (K, Na)AlSi<sub>3</sub>O<sub>8</sub>, is a potential host mineral of K in the deep mantle due to its stability [1] and abundance in high pressure phase assemblages of K-rich compositions [2]. Phase relations in the system KAlSi<sub>3</sub>O<sub>8</sub>-NaAlSi<sub>3</sub>O<sub>8</sub> are important in understanding the behavior of the hollandite solid solution under high pressure and high temperature, but it remains unclear whether the Na hollandite end member is a thermodynamically stable phase under some conditions or not. Previous studies reported that the maximal solubility of NaAlSi<sub>3</sub>O<sub>8</sub> in K hollandite was limited to 50 mol % [3,4], while most of hollandite found in meteorites contain a large amount of Na, 80-90 mol % [e.g. 5,6]. Some DAC experiments [7,8] identified trace NaAlSi<sub>3</sub>O<sub>8</sub> hollandite in laser-heated albite compositions by few fuzzy XRD peaks of hollandite, but the unsatisfactory XRD data and prevailing amounts of coexisting phases (CF NaAlSi<sub>0</sub>O<sub>4</sub> and stishovite) in the hollandite-containing product weaken the conclusion about the stability of NaAlSi<sub>3</sub>O<sub>8</sub> hollandite.

We investigated the phase relations in the system KAlSi<sub>3</sub>O<sub>8</sub>-NaAlSi<sub>3</sub>O<sub>8</sub> at pressures of 20-23 GPa and temperatures of 1873 and 2273 K. The obtained phase relations are modally consistent with those of the reference [3]: hollandite plus jadeite plus stishovite at relatively low pressures, hollandite plus the calcium ferrite type NaAlSiO<sub>4</sub> plus stishovite at relatively high pressures, and hollandite single phase when the Na content of the starting material is lower than the solubility of NaAlSi<sub>3</sub>O<sub>8</sub> in K hollandite at the corresponding condition. K hollandite dissolves more NaAlSi<sub>3</sub>O<sub>8</sub> component with pressure increase until the breakdown of jadeite at about 22 GPa, and the Na content in K hollandite decreases substantially with further increasing pressure. The solubility of NaAlSi<sub>3</sub>O<sub>8</sub> in K hollandite positively correlates with temperature, and it is very sensitive to both pressure and temperature around the pressure corresponding to the dissociation of jadeite. Hollandite with Na content of 50 mol % was recovered at 22 GPa and 1873 K, and Na-rich hollandite with 78 mol % Na was synthesized for the first time at 22 GPa and 2273 K. Lattice parameters of hollandite solid solutions decrease with increasing NaAlSi<sub>3</sub>O<sub>8</sub> component. The improved phase relations can be used to estimate the composition of hollandite in the Earth's interior. The positive temperature dependence of the NaAlSi<sub>3</sub>O<sub>8</sub> solubility in K hollandite and the synthesis of Na-rich hollandite suggest a stability region for NaAlSi<sub>3</sub>O<sub>8</sub> hollandite around 22 GPa at temperatures (slightly) higher than 2273 K, under which the formation of lingunite during meteorite impact can be elucidated via the phase equilibrium.

<sup>&</sup>lt;u>References</u>. [1] Hirao, N.et al. (2008): *Phys Earth Planet Inter*, **166**, 97-104; [2] Irifune, T. et al. (1994): *Earth Planet Sci Lett*, **126**, 351-368; [3] Yagi, A. et al. (1994): *Phys Chem Miner*, **21**, 12-17; [4] Liu, X. (2006): *Earth Planet Sci Lett*, **246**, 317-325; [5] Gillet, P. et al (2000): *Science*, **287**, 1633-1636; [6] Tomioka, N. et al. (2000): *Geophys Res Lett*, **27**, 3997-4000; [7] Liu, L. (1978): *Earth Planet Sci Lett*, **37**, 438-444; [8] Tutti, F. (2007): *Phys Earth Planet Inter*, **161**, 143-149.

#### **Direct Sound Velocity Measurements of Pyrolite Across the Mantle Transition Region**

S. Gréaux<sup>1,2</sup>, T. Irifune<sup>1,2</sup>, M. Nishi<sup>1</sup>, Y. Higo<sup>3</sup>, T. Inoue<sup>1</sup>, T. Arimoto<sup>1</sup>, Z. Liu<sup>1</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University, <sup>2</sup>Earth-Life Science Institute, Tokyo Institute of Technology, <sup>3</sup>SPring-8, JAMSTEC Corresponding author's email address: greaux@sci.ehime-u.ac.jp

Comparison of seismic data with laboratory sound wave velocities in minerals at high-pressure and high temperature plays a major role in interpreting the variations in composition as a function of depth in the Earth's interior. Although numerous studies have investigated the sound velocities of minerals under high pressure and high temperature (see a review by Li and Liebermann [1]), it is still debated that the pyrolite model explains well the seismic velocity profiles of seismological reference models. To this day, mantle velocities are estimated by averaging data from single phase studies [2], sometime using results from those using different techniques. In addition, only few of those experiments were conducted at pressure and temperatures relevant to the Earth's deep interior.

Here we investigated directly the velocities of pyrolite aggregates at pressures up to 30 GPa and temperatures up to 1700 K, which correspond to the lowermost part of the Earth's lower mantle. High pressure and high temperature sound velocities of pyrolite were measured by the ultrasonic interferometry method combined with synchrotron radiation techniques in a large volume press. Starting materials consisted of polycrystalline aggregates with a pyrolite bulk composition. Samples hot-pressed at 10 GPa consisted of Olivine (Ol), Garnet (Gt) and Pyroxenes (Px) while those synthesized at 17 GPa and 27 GPa respectively consisted of Wadsleyite (Wd) and Majorite garnet (Mj); and Bridgmanite (Br), Periclase (Pc) and CaSiO<sub>3</sub> perovskite (CPv).

We observed a clear contrast in between the velocities of the Ol+Gt+Px assemblage compared to those of Wd+Mj in agreement with the Olivine-to-Wadseleyite transformation at  $\sim$ 14 GPa [3]. The velocity gradients associated with phase transformations are well consistent with PREM [4] in the lowermost transition region but fail to explain its uppermost part especially at the 410 km depth discontinuity. Velocities at pressures higher than 25 GPa are also presented and the overall data discussed relative to the mineralogical composition of the mantle across the transition region.

<sup>&</sup>lt;u>References</u>. [1] Li, B. and Liebermann, R.C. (2014): *Phys. Earth Planet. Int*, **233**, 135-153; [2] Irifune, T. et al. (2008): *Nature*, **451**, 814-817; [3] Katsura, T. et al. (2004): *J. Geophys. Res. B*, **109**. [4] Dziewonski, A.M. and Anderson, D.L. (1981): *Phys. Earth Planet. Int*, **25**, 297-356.

#### Effects of the Subducted Slab on Dynamics of the Lowermost Mantle

## T. Kaneko, T. Nakakuki

Department of the Earth and Planetary Systems Science, Hiroshima University, Japan Corresponding author's email address: d154713@hiroshima-u.ac.jp

The structure and evolution of the Earth's lowermost mantle must be significantly influenced from subduced slabs, as seismological studies indicate that the slabs penetrate into the lower mantle. Seismological studies also suggest prominent features on the morphology (e.g. high elevation, steep edge [1], correlation between margin and hot spot locations [2]) and the stability (e.g. existence over a long term [2]) of the large low shear velocity provinces (LLSVPs) that exist at the base of the mantle. We perform a numerical study to investigate that influence of the lower mantle properties on the mechanical interactions of the subducted slab with a post-perovskite phase change and a compositionally dense layer by using a 2-D Cartesian model.

Our model simulates a whole mantle convection system in which plate-like motion is realized without any forces imposed on the lithosphere. Therefore we can observe the evolution of the lowermost mantle structure coupled with natural subducted slab behavior. We introduce a chemically distinct segment with the density increase of 77.3 kg m<sup>-3</sup> and the post-perovskite phase change with the Clapeyron slope of +8 MPa K<sup>-1</sup> and the density contrast of 49.9 kg m<sup>-3</sup>. We also incorporate phase diagrams of hydrous minerals [3] and hydration effects on the density and the viscosity [4]. In this study, we focus on the following parameters that affect the slab subducting history and the evolution of the dense layer; depth profile of the background mantle viscosity, depth dependence of a thermal expansivity and yield strength of the slab.

The viscosity profiles effects on not only the slab sinking velocity, but also temperature and deformation of the dense layer. The small viscosity of the lower mantle results in temperature increase in the whole potion of the chemically dense segment due to effective convection in the inside of the segment. Therefore, a thermal boundary layer is developed above the chemically dense segment. Moreover, the dense layer tends to significantly deform by strong mantle flow induced by the rapid subducted slab motion. When the lower mantle viscosity is as higher as  $10^{22}$  Pa s, the thermal boundary layer over the CMB, however, grows up without the development of small-scale convection in the dense layer. The slab yield strength has effects on the subducting slab structure when the thermal expansivity is constant. In the cases with the yield strength of 200 MPa, the subducting slab experiences buckling. The thermal expansivity plays important roles in the stability of the dense layer and a system of rising plumes. When the thermal expansivity is constant, the dense segment. On the other side, a thermal expansivity decreasing with depth stabilizes the dense structure. Furthermore, the upwelling plumes are generated on the top of the dense structure.

<sup>&</sup>lt;u>References</u>. [1] Ni, S. et al. (2002): *Sience*, **296**, 1850-1852; [2] Torsvik, T. H. et al. (2006): *Geophys. J. Int*, **167**, 1447-1460; [3] H. Iwamori. (2004): *Earth and Planetary Science Letters*, **227**, 57-71; [4] S. Karato. and H. Jung (2003): *Philosophical Magazine*, **83**, 401-414.

#### Single Crystal Elasticity of the Lower Mantle Minerals Using Inelastic X-ray Scattering

H. Fukui<sup>1,2</sup>, A. Yoneda<sup>3</sup>, A.Q.R. Baron<sup>2</sup>

<sup>1</sup>Graduate School of Material Science, University of Hyogo <sup>2</sup>Materials Dynamics Laboratory, RIKEN SPring-8 Center <sup>3</sup>Institute for Study of the Earth's Interior, Okayama University Corresponding author's email address: fukuih@sci.u-hyogo.ac.jp

Experimental study on single crystal elasticity of the earth's lower mantle materials is important to understand chemical and thermal structures of the earth's interior. Some synthesized samples of the lower mantle materials are tiny and opaque. Inelastic X-ray scattering technique is a powerful tool to investigate that property of these samples [1].

We have performed IXS measurements on CaIrO<sub>3</sub> with a *Cmcm* postperovskite structure [2] and (Mg,Fe,Al)(Si,Al)O<sub>3</sub> with a *Pbnm* perovskite structure [3] and revealed their full elastic stiffness matrices. The *Cmcm*-CaIrO<sub>3</sub> is an analogue material of *Cmcm*-MgSiO<sub>3</sub>, which is considered a main component of D" layer just above the Earth's core-mantle boundary. The diversity of elastic wave velocity in D" layer [4] can be explained from latticepreferred orientation and seismic anisotropy of the analogue material. We have experimentally found that cation substitution makes the single crystal elasticity of *Pbnm*-(Mg,Fe,Al)(Si,Al)O<sub>3</sub> more anisotropic and, makes bulk and shear moduli larger and smaller, respectively (Figure 1). This can explain the seismic anti-correlated anomaly observed in the deep lower mantle [5].



Figure 1. Stereo projections of elastic wave velocities of *Pbnm*-(Mg,Fe,Al)(Si,Al)O<sub>3</sub>, bridgmanite based on elastic stiffness constants determined by inelastic x-ray scattering. The crystallographic directions *a*, *b*, and *c* are shown in panel (a). The unit of scale bars in  $m \cdot s^{-1}$ . (a-c)  $V_P$ , average of two  $V_S$ , and difference between two  $V_S$ , respectively, for MgSiO<sub>3</sub> bridgmanite. (d-f) Those for Fe and Al bearing one.

<u>References</u>. [1] Fukui, H. et al. (2008): *Journal of Synchrotron Radiation*, **15**, 618-623; [2] Yoneda, A.et al. (2014): *Nature Communications*, **5**, 3453; [3] Fukui, H. et al.(*submitted*); [4] Lay, T. and Garnero, E. (2011): *Annual Review of Earth Planetary Science*, **39**, 91-123; [5] Trampert J. et al. (2004): *Science*, **306**, 853–856.

#### Thermal Equation of State of MgSiO<sub>3</sub> Post-perovskite

T. Sakai<sup>1</sup>, H. Dekura<sup>1</sup>, N. Hirao<sup>2</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University <sup>2</sup>Japan Synchrotron Radiation Research Institute Corresponding author's email address: sakai@sci.ehime-u.ac.jp

We established thermal equations of state (EoS) of MgSiO<sub>3</sub> post-perovskite phase determined both by laser-heated diamond anvil cell (LHDAC) and density-functional theoretical techniques. The LHDAC experiments were performed up to a pressure (P) of 265 GPa at temperature (T) of 300 K and 170 GPa at 2560 K. The *ab initio* calculations were performed up to 1.2 TPa and 6000 K. The Keane and AP2 equations of state models at multi-megabar range that include parameters at high-pressure limit to infinity were adopted for the first time to extract some meaningful physical properties. The volume data experimentally obtained in the wide pressure-temperature range were then applied to the Mie-Grüneisen-Debye model with fully experimental parameters. The Grüneisen parameter and its volume dependency were found consistent perfectly with the theoretically obtained ones. Both the experimental and theoretical EoSs are also found in very good agreement with each other within 0.1% in volume at the earth's core-mantle boundary condition, and the relation keeps within 0.8% even up to 300 GPa and 6000 K. Our newly developed EoSs should be applicable to the super-Earth's mantle as well as the Earth's core-mantle boundary region.

#### Experimental Identification of a New Pyrite-type Hydroxide at Multimegabar Pressures

M. Nishi<sup>1,2</sup>, Y. Kuwayama<sup>1,2</sup>, J. Tsuchiya<sup>1,2</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University <sup>2</sup>Earth-Life Science Institute, Tokyo Institute of Technology Corresponding author's email address: nishi@sci.ehime-u.ac.jp

The discovery of the new high pressure hydrous minerals has the important implications for the structure, dynamics and evolution of the Earth, since the hydrogen in the mantle has significant effects on the physical properties and stabilities of constituent minerals in the Earth. In order to understand the global circulation mechanism of hydrogen in the Earth, a number of high pressure experiments on hydrous phases have been conducted. The recent discovery of new hydrous minerals, phase H and  $\delta$ -AlOOH with very similar crystal structures, implies that the deep water subduction can reach to the bottom of the lower mantle. However, studies on the stabilities of hydrous minerals at pressures higher than those of the Earth's mantle have been scarce, in spite of their importance for exploring the potential presence and role of water in gigantic planets. In-situ X-ray diffraction experiments on AlOOH were performed using a laser-heated diamond-anvil cell (DAC) technique to investigate the stability and phase transition of hydroxide at high pressures. We succeeded to observe the phase transition of  $\delta$ -AlOOH to a pyrite-type structureat above 190 GPa and 2500 K with an increase in density of 2.6 %. The result is supported by first-principles density-functional calculations, which predict the pyrite-type AlOOH stabilizes at above 170 GPa. The stability of the pyrite-type hydroxide at the extreme high pressure may affect the modeling on the internal structure and deep water circle of some extra-solar planets.

#### Technical Developments in High Temperature Generation with Sintered Diamond Anvils

<u>T. Arimoto<sup>1</sup></u>, T. Irifune<sup>1,2</sup>, M. Nishi<sup>1,2</sup>, Y. Tange<sup>3</sup>, T. Kunimoto<sup>1</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University, <sup>2</sup>Earth-Life Science Institute, Tokyo Insitute of Technology, <sup>3</sup>JASRI Corresponding author's email address: arimoto@sci.ehime-u.ac.jp

Kawai-type multi-anvil apparatus (KMA) with sintered diamond (SD) anvils is a powerful apparatus to provide high pressure and high temperature condition corresponding to Earth's lower mantle. To date, a number of studies on the high pressure generation using SD anvils have been reported [e.g. 1, 2], and Yamazaki et al. (2014) achieved pressures up to 109 GPa. However, the high temperature generation corresponding to mantle geotherm over 50 GPa region has been quite difficult. In this study, we report recent works for technical developments in high temperature generation using SD anvils.

High pressure and high temperature experiments were carried out at BL04B1 beamline, SPring-8, and geodynamics research center, Ehime University. Two KMA (SPEED-Mk.II and MADONNA II) were used. SD anvils with TEL 1.5 mm were used. Pressure was calculated by the equation of state of gold [3], and temperature was monitored by a  $W_{97}Re_3-W_{75}Re_{25}$  thermocouple placed adjacent to a sample. A LaCrO<sub>3</sub> and a cylindrical Re were used as a heater.

We optimized the cell assembly for SD anvils in order to improve efficiency of pressure and temperature generations, and achieved the maximal pressure to 64 GPa at 6.0 MN. High temperature generation to 2000 K was made at 59 GPa. Performance of LaCrO<sub>3</sub> heater was quite stable without any scattering at that pressure region during 2 hours. On the other hand, the higher temperature generation (2773 K) using Re heater was reported by Ito et al. (2004) [4]. Therefore, we additionally tested the Re heater combined with assembly for SD anvils.

<u>References</u>. [1] D.Yamazaki et al. (2014): *Phys Earth Planet. Inter*, **228**, 262-267; [2] Y.Tange et al. (2008): *High Pres. Res*, **28**, 245-254; [3] T. Tsuchiya. (2003): *J. Geophys. Res*, **108**, B10, 2462; [4] E. Ito et al. (2004): *Phys Earth Planet. Inter*, **143-144**, 397-406.

#### Over 3000°C Generation in Kawai-Cell Byboron-Doped Diamond Cylinder Heater

#### L.J. Xie, Akira Yoneda, Eiji Ito

Institute for Study of the Earth's Interior, Okayama University Corresponding author's email address: p1f77h4y@s.okayama-u.ac.jp

It is the first report of synthesizingsemi-conductor boron-doped diamond (BDD) cylindrical heaterin the Kawai-type multi-anvil apparatusat 15 GPa and 2100°C. The dimension of the cylindrical heaters was2.6/1.5/3.35 mm in order of outer diameter, inner diameter, and length.SEM image shows that the grain size of diamond is about 1  $\mu$ m.

The cylindrical heater wastested for extremely high temperature generation in a large sample volume ( $\sim 0.1 \text{mm}^3$ ) in the Kawai apparatus; the sample volume is  $\sim 1000$  times larger than that in diamond anvil cell. This work was the first trial of pre-synthesized BDD heater in Kawai-type apparatus. The reproducibility of the BDD heater was confirmed well through three times of repeated cycles of heating and cooling. The BDD heater with 3 wt.% boron showed metallic behavior, i.e. increasing resistance with increasing temperature. This electrical characteristic was beneficial forstable generation of temperature as high as up to 2700°C; the heating for further higher temperature was failed owing to the deterioration of electrode.

We succeeded to generate temperature up to ~3500 °C by using a smaller BDDheater (1.5/1.0/6.0 mm) and TiC electrode. We molded this heater from BDD powder to overcome the difficulty synthesizing such a thin BDD cylinder at high pressure. Temperatures higher than 1800 °C were estimated from the input power based on its power-temperature relationshipbefore ofthermocouple. The effect of hard BDD heater onpressure the break the generationwasexamined in the *in-situ* X ray experiment at SPring-8.

BDD heateris free from complicated power-temperature relationship and pressure drop associated with graphite-diamond conversion. Thus it is much more advantageous than boron doped graphite heater.

#### **Properties of Liquid Iron Alloys under Extreme Conditions**

<u>G. Morard<sup>1</sup></u>, D. Andrault<sup>2</sup>, D. Antonangeli<sup>1</sup>, J. Siebert<sup>1</sup>, F. Guyot<sup>1</sup>, A.L. Auzende<sup>1</sup>, O. Lord<sup>3</sup>, J.Bouchet<sup>4</sup>, M.Harmand<sup>1</sup>, B.Cochain<sup>5</sup>, G.Garbarino<sup>6</sup>, I.Kantor<sup>6</sup>, R.Torchio<sup>6</sup>, E.Boulard<sup>6</sup>, M.Mezouar<sup>6</sup>

 <sup>1</sup>IMPMC. CNRS. Université Pierre et Marie-Curie, Paris, France
 <sup>2</sup>Laboratoire Magmas et Volcans, Clermont-Ferrand, France
 <sup>3</sup>School of Earth Sciences, University of Bristol, Wills Memorial Building, Queen's Road, Bristol, BS8 1RJ, UK
 <sup>4</sup>CEA, DAM, 91297 Arpajon, France
 <sup>5</sup>Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy Centre for Science at Extreme Conditions (CSEC) University of Edinburgh, Edinburgh, EH9 3JZ, UK
 <sup>6</sup>European Synchrotron Radiation Facility, Grenoble, France

Corresponding author's email address: guillaume.morard@impmc.jussieu.fr

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

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

#### Liquid Iron Alloys with Hydrogen at Outer Core Conditions by First Principles

K. Umemoto<sup>1</sup>, K. Hirose<sup>1,2</sup>

<sup>1</sup>Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo, Japan <sup>2</sup>Laboratory of Ocean-Earth Life Evolution Research Japan Agency for Marine-Earth Science and Technology, Kanagawa, Japan Corresponding author's email address: umemoto@elsi.jp

Since the density of the outer core deduced from seismic data is about 10% lower than that of pure iron at core pressures and temperatures (P-T), it is widely believed that the outer core includes one or more light elements. Although intensive experimental and theoretical studies have been performed so far, the light element in the core has not yet been identified. Comparison of the density and sound velocity of liquid iron alloys with observations, such as the PREM, is a promising way to determine the species and quantity of light alloying component(s) in the outer core. Here we report the results of a first-principles molecular dynamics study on liquid iron alloyed with hydrogen, one of candidates of the light elements. Hydrogen had been much less studied than other candidates. However, hydrogen has been known to reduce the melting temperature of Fe-H solid [1]. Furthermore, very recently, Nomura et al. argued that the outer core may include 24 at.% H in order to be molten under relatively low temperature (< 3600 K) [2]. Since then hydrogen has attracted strong interests. We clarify the effects of hydrogen on density and sound velocity of liquid iron alloys under outer core P-T conditions. It is shown that ~1 wt% hydrogen can reproduce PREM density and sound velocity simultaneously very well. In addition, we show the presence of hydrogen rather reduces Grüneisen parameters. It indicates that, if hydrogen exists in the outer core, temperature profile of the outer core could be changed considerably from one estimated so far.

<u>References</u>. [1] Sakamaki, K. et al. (2009): *Phys. Earth Planet. Inter*, **174**, 192-201; [2] Nomura, R. et al. (2014): *Science*, **31**, 522-525.

#### **Core Liquids: Fact and Fiction**

#### G. Helffrich

## Earth-Life Science Institute, Tokyo Institute of Technology Corresponding author's email address: george@elsi.jp

The heat flowing through the core-mantle boundary is a control on the conditions for convection in the mantle [1] and for the cooling of the core from its initial stateand development of its dynamo [2]. Recent work on measuring core metal transport properties at high pressures and temperatures [2] shows that the core transfers heat more readily than the best-guess extrapolations from ambient conditions, and poses problems for the long-term viability of the geodynamo as it operates today. One remedy is that long-term core stratification reduces the heat transfer rate due to thermal or chemical stratification. This prolongs the growth of the inner core allowing a dynamo by release of chemical buoyancy at the inner core boundary.

There is evidence that parts of the outer core are not in a well-mixed, adiabatic state, particularly the top of the core where heat transfer to the mantle takes place [3]. Some view this evidence as controversial because it does not correspond to their belief that adding any light element to iron liquid necessarily raises seismic wavespeeds [4]. This belief is buttressed by first principles calculations of liquid iron alloy wavespeeds that uniformly show rising seismic wavespeeds with rising light element concentration [5]. However, experimental data for iron-sulfur mixtures unequivocally show that seismic wavespeeds decrease as more sulfur is added. Hence the prevailing belief needs revision in the face of actual data. To advance understanding of the core's properties and of Earth evolution, we need to pursue a market basket of approaches that are anchored to observational data rather than beliefs. I outline one approach interpreting the seismic wavespeed variations in the top of the outer core.

<sup>&</sup>lt;u>References</u>. [1] Labrosse, S. et al. (2007): *Nature*, **450**, 866-869; [2] Gomi, H. et al. (2013): *Phys. Earth and Planet. Int*, **224**, 88-103; [3] Helffrich, G. & Kaneshima, S. (2010): *Nature*, **468**, 807-810; [4] Buffett, B. & Seagle, C. (2010): *J. Geophys. Res*, 115; [5] Badro, J. et al. (2013): *Proc. Nat. Acad. Sci*, **111**, 7542-7545.

#### Crystallization of SiO<sub>2</sub> in Earth's Core after High-temperature Core Formation

 $\frac{\text{K. Hirose}^{1}, \text{G. Morard}^{2}, \text{H. Ozawa}^{3}, \\ \text{G. Helffrich}^{1}, \text{J. Hernlund}^{1}$ 

<sup>1</sup>Earth-Life Science Institute, Tokyo Institute of Technology <sup>2</sup>IMPMC, Universite Pierre-et-Marie-Curie, <sup>3</sup>Okayama University

Recent core formation models based on the metal-silicate partitioning of siderophile elements suggest that the Earth's core was formed by metal segregation from silicate at high pressure and high temperature in a deep magma ocean. It is also known that the simultaneous solubility of silicon and oxygen in liquid iron are strongly enhanced at high pressure and high temperature, such that at the end of accretion the core was rich in both silicon and oxygen. Here we performed crystallization experiments on the Fe-Si binary and Fe-Si-O ternary systems up to core pressure in a laser-heated diamond-anvil cell. Thestarting material for the latter was a homogeneous mixture of fine-grain Fe-Si and SiO<sub>2</sub> (<1µm). We prepared cross sections of samples recovered from the DAC using a focused ion beam (FIB) and subsequently performed textural and chemical characterization with field-emission-type electron microprobe (FE-EPMA). Quenched liquid alloy was found at the hottest part coexisting with a solid phase (liquidus phase) at theperiphery. These results combined with literature data on the melting phase relations in the Fe-FeO binary system demonstrate that the liquidus field of SiO<sub>2</sub> is very wide at the Fe-rich portion of the Fe-Si-O ternary system at the core pressure range. It indicates that the original Fe-Si-O core liquid should have crystallized a large amount of SiO<sub>2</sub> until it lost either silicon or oxygen. The recent finding of high thermal conductivity of the core suggests that core thermal convection is difficult to sustain without extreme degrees of secular cooling. However, even for modest degrees of joint Si-O incorporation into the early core, the buoyancy released by crystallization of SiO<sub>2</sub>issufficient to overcome thermal stratification and sustain the geodynamo.

## Linking Seismic Observations of Earth's Inner Core Boundary to Deeper Structure

L. Waszek<sup>1</sup>, A. Deuss<sup>2</sup>, H. Godwin<sup>3</sup>

## <sup>1</sup>University of Maryland College Park, <sup>2</sup>University of Utrecht, <sup>3</sup>University of Oxford Corresponding author's email address: lauren.waszek@cantab.net

The inner core boundary marks the phase transition between the solid inner core and the fluid outer core. As the site of inner core solidification, the boundary provides insight into the processes generating the seismic structures of the inner core. In particular, it may hold the key tounderstanding the previously observed hemispherical asymmetry in inner core seismic velocity, anisotropy and attenuation. Here, we use a large PKiKP-PcP amplitude ratio and travel timeresidual dataset to investigate velocity and density contrast properties near the inner coreboundary. Although hemispherical structure at the boundary has been proposed by previousinnercore studies, we find no evidence for hemispheres in the amplitude ratios or travel time residuals.

The amplitude ratios are much larger than predicted, and show no regional coherency, while thetravel time residuals display large regional variations.Beneath the inner core boundary, previous studies have constrained the hemispherical seismicvelocity structure in the Earth's inner core at depths greater than 15 km below the inner coreboundary. However, the properties of shallower structure have not yet been determined, because the seismic waves used for analysis arrive close together and interfere. The uppermost layer of the inner core was formed most recently, thus is most strongly correlated to the inner coresolidification processes and structures at the inner core boundary. To study this upper region, we present a new waveform modeling method to measure the seismic velocity in the top 15 km of the inner core. As proof of concept, we apply our method to an event with ray paths which traverse the Pacific hemisphere boundary. Our preliminary observations indicate hemispherical structure in the uppermost layers of the inner core, despite no hemispherical structure at the boundary itself.

#### **Freezing and Melting above the Inner Core Boundary**

M. Lasbleis<sup>1</sup>, J. Hernlund<sup>1</sup>, S. Labrosse<sup>2</sup>

## <sup>1</sup>Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo <sup>2</sup>Laboratoire de Géologie de Lyon, ENS de Lyon, France Corresponding author's email address: marine.lasbleis@elsi.jp

Seismic observations of the Earth's core reveal a complex structure: radial and lateral heterogeneities in seismic anisotropy and attenuation in the solid inner core, but also discrepancies between observed P-wave velocity and homogeneous PREM model in the deep liquid outer core. [1] showed that no published large-scale dynamical model can explain the whole complexity of the inner core, as seen by the seismic observations. Here we want to focus on the freezing and melting processes that occur at the inner core boundary and above.

In particular, the 200km anomalous layer at the bottom of the outer core exhibits seismic velocities lower than the PREM model. It has been interpreted as a layer depleted in light elements, whereas the usual model considers that light elements are expelled at the surface of the inner core by freezing of the outer core alloy. Recent models of core formation argued for an early stratified liquid core, and the stratified layers at the top and bottom of the outer core would be a vestige of this primordial stratification. However, freezing of the inner core at the inner core boundary releases light elements that provide buoyancy fluxes that would mix the stratified liquid above with small-scale buoyant plumes. To model the F-layer, we consider that the freezing of the iron alloy and the release of light elements have to occur in the bulk of the layer. Iron snow forms and settles in the layer, buffering the thermal and chemical profile to the liquid. We show that this dynamics can both sustain and stabilise the stratified layer in the liquid outer core while simultaneously matching the seismic observations.

References. [1] Lasbleis, M., & Deguen, R. (2015): Physics of the Earth and Planetary Interiors.

#### Thermal Structure of the Inner Core Boundary in Numerical Dynamos

#### H. Matsui

## Department of Earth and Planetary Sciences, University of California, Davis Corresponding author's email address: hrmatsui@ucdavis.edu

Seismic anisotropy through alignment of crystal lattices suggests aspherical growth of the inner core. Slow viscous deformation of the inner core and latent heat distribution by flow motion are expected to be the origin of the aspherical growth of the inner core. In Buffett and Matsui (2015)[1], the temperature heterogeneity at ICB was prescribed and investigated a change of largescale flow due to this heterogeneity. In the present study, we solve magnetohydrodynamics (MHD) simulation in a rotating spherical shell with considering the heat equation in the inner core. To compare the results with the simulation without considering the inner core, we assume that the inner core is electrically insulated and co-rotate with mantle. In addition, we set the same thermal diffusivity for the inner core and outer core, and introduce a constant heat source in the inner core to keep the average temperature in the outer core through the simulations. We also set a homogeneous heat flux at the outer boundary of the shell as a thermal boundary condition at CMB. We compare the simulations results with the simulations results using fixed heat flux or temperature condition at ICB.

The results show that larger temperature heterogeneity is generated than the heat flux at ICB because heat flux at ICB has smaller length and time scale comparing with the temperature variation at ICB. In these results, a large temperature variation is observed at the both ICB and CMB. The range of the variation is approximately 0.9 times of the average temperature difference between ICB and CMB. The largest temperature variation is observed in  $Y_2^0$  component in the spherical harmonics. i.e., higher and lower temperature is observed at the poles and equator, respectively. This temperature pattern at ICB also reflects the temperature pattern at CMB. We observe the high temperature patch at the pole, while lowest temperature is observed in the fixed temperature ICB case. On the other hand,  $Y_1^1$  component, which can generate a transition mode in the inner core, is approximately 0.1 times of the  $Y_1^1$  component and drifts in the zonal direction for approximately a half of the magnetic diffusion time. Consequently,  $Y_2^0$  component remains as a stable temperature heterogeneity at ICB.

We do not take into account for the latent heat in the present simulations. Constructing a model including the latent heat at ICB will be the next study. We expect that the latent heat will stabilize the temperature heterogeneity at ICB in the present study. However, present results will be good reference to compare the model with the latent heat.

References. [1] Buffett, B.A, and Matsui, H. (2015): Physics of the Earth and Planetary Interiors, 243, 22-29.

#### Lattice Preferred Orientation of Hcp-Iron Induced by Shear Deformation

<u>Y. Nishihara</u><sup>1</sup>, T. Ohuchi<sup>1</sup>, T. Kawazoe<sup>1,2</sup>, G. Maruyama<sup>1</sup>, Y. Higo<sup>3</sup>, K. Funakoshi<sup>3,4</sup>, Y. Seto<sup>5</sup>

<sup>1</sup>Geodynamics Research Center, Ehime University, <sup>2</sup>BGI, Bayreuth University <sup>3</sup>JASRI, <sup>4</sup>CROSS-Tokai, <sup>5</sup>Kobe University Corresponding author's email address: yunishi@ehime-u.ac.jp

Many hypotheses have been proposed for origin of seismic anisotropy in the Earth's inner core which consists of solid metal. Plastic deformation of constituent material (most probably hexagonal-close-packed (hcp) iron) is one of the candidate processes to form the inner core anisotropy (e.g. [1]). Thus knowledge of deformation-induced lattice preferred orientation (LPO) of hcp-iron is important for understanding of nature of the inner core. Only limited numbers of experimental studies have been reported on deformation induced LPO of hcp-iron because this phase is unquenchable to ambient condition. In the previous studies, hcp-iron was deformed by uniaxial compression, and slip activities in deforming sample were indirectly estimated based on elastoplastic self-consistent modeling (e.g. [2]). In this study, we have carried out shear deformation experiments on hcp-iron and determined its deformation induced LPO.

Shear deformation experiments of hcp-iron were carried out at pressure of 9–18 GPa and temperature of 723 K using a D-DIA apparatus, SPEED-Mk.II-D, installed at BL04B1, SPring-8 [3]. In the deformation experiments, pressure medium of 4.5 or 5.0 mm (Mg,Co)O cube and WC and cBN second stage anvils with 2.5 or 3.0 mm truncation were used. The sample iron was sandwitched between two 45°-cut Al<sub>2</sub>O<sub>3</sub> pistons in the cell assembly. Shear strain rates in the experiments were  $\sim 2 \times 10^{-4}$  or  $\sim 0.6 \times 10^{-4}$  s<sup>-1</sup>, and total shear strain is  $\sim 2$ . Development of LPO in the deforming sample was observed in-situ based on two-dimensional X-ray diffraction using an imaging plate detector and monochromatized synchrotron X-ray with energy of 49–51 keV. LPO of sample was determined from the two-dimensional diffraction pattern using a software ReciPro 2 [4].

In shear deformation of hcp-iron,  $\langle 0001 \rangle$  and  $\langle 11\bar{2}0 \rangle$  axes gradually aligned to be sub-parallel to shear plane normal and shear direction, respectively, from initial random orientation. The  $\langle 0001 \rangle$  and  $\langle 11\bar{2}0 \rangle$  axes are back-rotated from shear direction by  $\sim 30^{\circ}$ . The above results suggest basal slip  $\langle 11\bar{2}0 \rangle \{0001\}$  is the dominant slip system under the studied deformation conditions. It has been shown that Earth's inner core has an axisymmetric anisotropy with P-wave traveling  $\sim 3\%$  faster along polar paths than along equatorial directions. Although elastic anisotropy of hcp-iron at the inner core conditions is still controversial, recent theoretical studies consistently shows that P-wave velocity of hcp-iron is fastest along  $\langle 0001 \rangle$ direction at least at low-temperatures. Our experimental results could be suggesting that most part of the inner core deforms with shear plane sub-parallel to equatorial plane (e.g. [5]).

<sup>&</sup>lt;u>References</u>. [1] Sumita, I & Bergman, M.I. (2009): *Treatise on Geophysics***8**, *Core Dynamics*, 299-318; [2] Merkel, S., *et al.* (2004): *Phys. Earth Planet. Int*, **145**, 239-251; [3] Kawazoe, T. *et al.* (2011): *Am. Mineral*, **96**, 1665-1672; [4] Seto, Y. (2012): *Rev. High Press. Sci. Tech*, **22**, 144-152; [5] Wenk, H.-R. *et al.* (2000): *J. Geophys. Res*, **105**, 5663-5677.

#### View and Perspectives on the Lower Mantle from Geo-neutrinos

## <u>S.T. Dye</u><sup>1,2</sup>

## <sup>1</sup>Department of Physics and Astronomy, University of Hawaii, Honolulu, HI 96822, USA <sup>2</sup>Department of Natural Sciences, Hawaii Pacific University, Honolulu, HI 96814, USA Corresponding author's email address: sdye@phys.hawaii.edu

We explore the capacity for geo-neutrino observations to estimate the quantity and distribution of radiogenic elements in the lower mantle. Geo-neutrinos originate as electron antineutrinos from the beta-minus decays of <sup>40</sup>K and of daughter nuclei in the decay series of <sup>232</sup>Th, <sup>238</sup>U, and <sup>235</sup>U. The long lifetimes of these isotopes make potassium, thorium, and uranium the main radiogenic, heat-producing elements in Earth. Neutrino emission from beta decay is isotropic, and neutrinos of all types carry no electric charge, allowing direct passage through electric and magnetic fields. Neutrino particle states have different masses, producing harmonic fluctuations of neutrino interaction states along the direction of travel. Because the wavelength of geo-neutrino oscillations is short compared with the size of geological reservoirs, an approximately constant reduction in the surface flux applies. The direction and energy spectrum of the geo-neutrino flux at the surface provide a unique, model-independent image of radiogenic reservoirs within Earth. Sufficient exposure of detectors, sampling over the surface of Earth, provides neutrino emission tomography of the planet. Geo-neutrino interactions with mater are extremely rare, requiring well-shielded, massive, and long-term detector projects in deep underground, and potentially underwater, locations.

Two inaugural underground detectors, one in Japan and one in Italy, are sampling the energy spectrum but not the direction of the geo-neutrino flux. In addition to geo-neutrinos, these detectors measure antineutrinos from nuclear reactors. Reactor antineutrinos are a dominant source of background to the geo-neutrino signal. The reported observations from the two detectors are consistent with one another, providing no model-independent evidence for the existence of geological reservoirs with different concentrations of radiogenic elements.

Estimating the quantity and distribution of radiogenic elements in the lower mantle by geo-neutrino measurements is a formidable task. It is probably most directly realized by geo-neutrino observations in the deep ocean and by developing the capability to measure the direction of the geo-neutrino flux. We discuss these possible achievements, describe recent progress on modeling the reactor antineutrino background, and present observational strategies for gaining perspective on the lower mantle.

#### **Geo-neutrino Measurement with KamLAND and Future Prospects**

#### H. Watanabe

Research Center for Neutrino Science, Tohoku University, 6-3 Sendai, Miyagi, 980-8578, JAPAN Corresponding author's email address: hiroko@awa.tohoku.ac.jp

The KamiokaLiquid-scintillator Anti-Neutrino Detector (KamLAND) is located in a rock cavern in the Kamioka mine, 1,000 m below the summit of Mt. Ikenoyama in Japan. KamLAND is marked by the ability to detect low-energy anti-neutrino signals at 1,000 tons of ultra pure liquid scintillator (LS) through the inverse  $\beta$  reaction,  $\bar{v}_e + p \rightarrow e + n$ . We demonstrated the oscillation nature of neutrino flavor transformation by observing electron anti-neutrino ( $\bar{v}_e$ ) from nuclear reactors and neutrino properties have been explored precisely [1,2]. Since neutrinos interact with other particles only via weal interaction, they have extremely low reaction probabilities. Such elusive property of neutrinos provides us with the ability to investigate optically invisible deep interior of the astronomical objects, such as the Earth. Neutrino measurement evolved understanding of neutrino properties to utilization of neutrino as a "probe".

The detection of geo-neutrinos,  $\bar{\nu}_e$ 's produced in  $\beta$ -decays from primordial radioactivite elements (uranium, thorium and potassium) within the Earth's interior, brings unique and direct information about the Earth's interior and thermal dynamics.KamLAND detects geo  $\bar{\nu}_e$  signals above



1.8 MeV due to the reaction threshold energy of the inverse  $\beta$ -decay, resulting to have sensitivity to  $\bar{v}_e$ 's from the decay chains of <sup>238</sup>U and <sup>232</sup>Th. The KamLAND collaboration reported the result of the first study of geo  $\bar{v}_e$  in 2005 [3]. Later the geo  $\bar{v}_e$  signals at KamLAND were used to estimate our planet's radiogenic heat production and constrain composition models of the bulk silicate Earth (BSE) [4]. Following the Fukushima nuclear accident in March 2011, the entire Japanese nuclear reactor industry, which generates >97% of the reactor  $\bar{v}_e$  flux at KamLAND, has been subjected to a protracted shutdown. This unexpected situation allows us to improve the sensitivity for geo  $\bar{v}_e$ 's [5].

Currently, geo  $\bar{\nu}_e$  observed rate is in agreement with the prediction from existing BSE composition models within  $2\sigma C.L.$ , but some extreme models start to be disfavored. This ability to discriminate is limited by the experimental uncertainty and crust modeling. Continuing the data taking under the present low-reactor situation yields better signal-noise ratio and provides promising power of uncertainty (21%[5]  $\rightarrow$  15% with 5-year measurement). Enhanced geo  $\bar{\nu}_e$  flux calculation model using latest crustal structure model and geochemical understanding around Japan Island Arc will be a key issue for the further constraint on the Earth models and observation of mantle contribution.

The directional measurement of incoming geo  $\bar{v}_e$ 's can map out the U and Th distribution inside the Earth and this new technic is also applicable to resolving crust versus mantle flux contribution. Our experimental studies and Monte-Carlo simulations confirmed that a combination of <sup>6</sup>Li-loaded LS and imaging detector has the feasibility of developing direction sensitive detector [6]. This new technology will open a new era of understanding of the Earth. <u>References</u>. [1] Eguchi, K. *et al.* (2003): *Phys. Rev. Lett*, **90**, 021802; [2] Araki, T. *et al.* (2005): *Phys. Rev. Lett*, **94**, 081801; [3] Araki, T. *et al.* (2005): *Nature*, **436**, 499; [4] Gando, A. *et al.* (2011): *Nature Geosci*, **4**, 647; [5] Gando, A. *et al.* (2013): *Phys. Rev. D*, **88**, 033001; [6] Tanaka H.K.M and Watanabe H. (2014): *Scientific Report (Nature)*, **4**, 4708.

#### **Core and Mantle Compositions: Neutrino Geophysics Insights**

#### W.F. McDonough

Geology, University of Maryland, College Park, MD 20742, USA Corresponding author's email address: mcdonoug@umd.edu

The Earth's four most abundant elements, O, Fe, Mg and Si, make up more than 90% of its mass; with the addition of Ni, Ca, Al, and S, we describe more than 98% the mass of the planet, including specifying the core's and mantle's compositions. The solar photosphere's composition validates the underlying assumption-chondritic meteorites provide a guide to planetary models.

There is no fixed amount of metal accreted or Mg/Si ratio for chondrites. Variations in this ratio reflect the proportion of olivine (2:1 molar Mg/Si) to pyroxene (1:1 molar Mg/Si) accreted in the planet or chondritic parent body. Astromineralogy studies increasingly reveal variations in the proportion of olivine to pyroxene in accretion disks, some with inner disk regions richer in olivine relative to the disk wide composition.

Core compositional models remain poorly constrained, with models assuming dissolved O, Si and S in the Fe-Ni-liquid. However, the relative and absolute abundances of light element(s) in the core remain elusive. There is no compelling reason to have heat producing elements (HPE) in the core; lower limit concentration estimates of HPE in the core are being established.

The upper and lower mantle are regarded as having similar compositions, with seismic tomography revealing upwelling plumes and downgoing slabs traversing the complete volume of the mantle, requiring lower-upper mantle mass exchange and mixing. A compositionally anomalous Earth is no longer tenable given the Earth's <sup>142</sup>Nd-isotopic composition overlaps with that observed in chondritic meteorites.

The Earth's geoneutrino signal allows us to directly assess the amount and distribution of Th and U inside the Earth and define the planetary budget of these refractory lithophile elements, and hence the amount of Ca and Al inside the Earth, which in turn defines the Ca-perovskite content of the lower mantle and from that the proportions of bridgmanite and ferropericlase [1-3]. Models of SiO<sub>2</sub>-enriched lower mantle are disfavored by the recent geoneutrino result [2], whereas pyrolytic



models and Ca-perovskite-rich models fall within the 1s limits of these results. The lower mantle has, on average by volume, about 10% Ca-perovskite, 17% ferropericlase, 73% bridgmanite [4]. Variations in the electron density of the Earth's interior can be probed by neutrino oscillation studies [5-6] using next-generation detectors. Results from these experiments will evaluate the hydrogen content of the core and later, with increasing data, will test specific compositional models of the relative proportions of O, Si and S dissolved in the metallic liquid alloy. The future is bright given developments in ocean-going detectors [7] and directionality technology [8]; *Particle Geoscience* will transform our understanding of the Earth's composition and structure.

References. [1] Usman, S.M. et al. (2015): Scientific Report (Nature), **5**,13945; [2] Agostini, M. et al. (2015): *Physical Review D*, **92**, 031101(R); [3] Gando, A. et al. (2013): *Physical Review D*, **88**, 033001; [4] McDonough, W.F. (2015): in *Deep Earth: Physics and Chemistry of the Lower Mantle and Core* (eds., Terasaki, H. & Fischer, R.); [5] Ioannisian, A.N. et al. (2015): *Physical Review D*, **92**, 013014; [6] Rott, C. et al. (2015). [7] Dye, S.et al. (2015): *Physics Procedia*, **61**, 310-218; [8] Tanaka, H.K.M. and Watanabe, H. (2014): *Scientific Report (Nature)*, **4**, 4708.