Lattice diffusion in B2-type MgO

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High-pressure and high-temperature rheology is essential for understanding the dynamics in planets. Diffusion creep might be one of the dominant viscoplastic mechanisms and lattice diffusion coefficient $D$ is a key property in this deformation process (e.g., Karato, 2011). Experimental measurements of $D$ however still remain technically difficult under deep planetary conditions. Theoretical approaches therefore play a substantial role.

B2 (CsCl)-type MgO is a high-pressure phase of B1 (NaCl)-type MgO and expected to be one of the major constituents in super-Earths' mantle and giant planetary core (Guillot, 1999; Tsuchiya and Tsuchiya, 2011). Although diffusion creep viscosity of super Earths’ mantle is usually assumed to increase with depth monotonically, a previous study (Karato, 2011) suggested that it could decrease associated with the B1-B2 transition of MgO. However, this idea is obtained based on measured plasticity of analog materials and thus $D$ of actual B2-type MgO is still underdetermined.

In this study, we calculate $D$ of B1- and B2-type MgO based on first principles constant-temperature molecular dynamics method combined with static lattice energy calculations. We identify distinctly larger $D$ of both Mg and O in B2-type than in B1-type at the same pressure, suggesting that B2-type would be less viscous as expected. The mechanisms of increase in $D$ will be presented.

Keywords: Lattice diffusion, First principles calculation, Super Earth
Microstructural development in olivine aggregates during dislocation creep under hydrous conditions

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Since hydrogen plays an important role in dynamic processes in the mantle, we conducted high-strain torsional shear experiments on aggregates of Fe-bearing olivine [(Mg,Fe)₂SiO₄; Fo50] under hydrous condition. Olivine with a composition of Fo50 was used because of its enhanced grain growth kinetics and low strength relative to Fo90. Two pieces of an oriented San Carlos olivine crystal were embedded in each aggregate to monitor water fugacity both before and after deformation. We deformed samples to high enough shear strain≈ 5, to achieve a steady-state microstructure. A non-linear, least-squares fit to the stress versus strain rate data yielded a stress exponent of $n \approx 3.5$, indicative of deformation involving dislocations. The water content determined from Fourier transform infrared (FTIR) spectroscopy analyses of the single crystals demonstrated that the samples were water saturated after deformation. Fabric analyses of the polycrystalline olivine samples, determined using electron backscatter diffraction (EBSD), indicate that the strength of the lattice preferred orientation (LPO) increases with increasing strain. Further, the LPO of olivine changes as a function of strain due to competition among three slip systems: (010)[100], (100)[001], and (001)[100]. Observed strain weakening can be attributed to geometrical softening due to LPO development, which reduces the stress by ~1/3 from its peak value in constant strain rate experiments. The evolution of fabric can be applied to investigations of upper mantle seismic anisotropy especially in a mantle wedge or in a shear zone, locations in which hydrous conditions prevail.

Keywords: olivine, high strain deformation, dislocation creep, geometrical softening due to LPO development
Differences in grain growth kinetics between MORB and pyrolitic materials under lower mantle conditions: preliminary results

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Convective mixing and persistence of chemical heterogeneities such as subducting slabs in the lower mantle largely depends on their density and viscosity contrasts. In contrast to detailed studies on the density, those on the viscosity of deep slab materials have been limited so far due to difficulties of direct quantitative deformation experiments. Previous studies suggest that both MORB and peridotite regions of deep slabs across the upper and lower mantle boundary cause significant grain-size reduction through the post-spinel and post-garnet transformations, respectively, resulting that the grain-size sensitive creep becomes dominant as the deformation mechanism (e.g., Kubo et al., PEPI2008; EPSL2009; AGU2011). Therefore, the grain growth is an important process controlling the viscosity of slab materials in the lower mantle. Here we report preliminary results on grain growth experiments of MORB and pyrolitic materials under lower mantle conditions.

Each material consists of 3-4 phases after the transformations; those are Mg-perovskite, Ca-perovskite, stishovite, and aluminous phase in MORB, and Mg-perovskite, Ca-perovskite, and ferropericlase (+majoritic garnet at the top of the lower mantle) in pyrolite. We conducted grain growth experiments in these assemblages using a Kawai-type multi-anvil apparatus at ~25-28 GPa, 1873-2373K, and for 1-600 min. SEM observations of recovered samples revealed that these assemblages exhibit relatively homogeneous equi-granular texture except for the short-duration annealing in the pyrolitic material. At the present stage, the average grain size was measured without distinction among phases in the case of MORB material, whereas the grain size in each phase was measured for the pyrolitic material. Preliminary analysis on the grain growth data indicates that the grain growth exponent is about 3.5 for both the MORB material and the major phase of Mg-perovskite in the pyrolitic material, suggesting that the grain growth kinetics in these multi-phase assemblages are controlled by an Ostwald ripening process. The grain size in the MORB material is smaller than that in the pyrolitic material, which corresponds to the difference of 100-150K in temperature. The difference in grain size evolution may lead to the viscosity contrast between MORB and pyrolitic materials in the lower mantle, however further detailed studies are needed to assess this issue.
In-situ X-ray diffraction measurement of growth kinetics of reaction rim at high pressures

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Diffusion rates of elements in minerals provide important constraints for understanding many physical and chemical processes in the Earth’s interior, including mantle rheology and chemical transportation. Therefore, many researchers showed the experimental studies on the growth kinetics of reaction rims between minerals, which are often controlled by diffusion of elements. Most of the previous studies succeeded to determine the rim growth kinetics based on the direct measurement of the thickness of reaction layers of recovered samples. However, it is difficult to obtain the precise growth kinetics in this method due to the small uncertainty of temperature and water contents during each experiment.

Here we use in situ X-ray measurements in conjunction with a multi-anvil apparatus to obtain the precise kinetic data of the rim growth of MgAl₂O₄ spinel between MgO periclase and Al₂O₃ corundum. Time resolved X-ray diffraction patterns enable us to obtain the information with the constant temperature, pressure, and water contents.

We succeeded to obtain the time-resolved X-ray diffraction data during the rim growth of MgAl₂O₄ spinel. However, the obtained growth kinetics contains large uncertainty because of the grain growth of the sample minerals due to high water contents. Further experimental improvement would be required to obtain the precise growth rate of the reaction rims.

Keywords: rim growth kinetics, mantle, multi-anvil apparatus
Effect of the metallic melt on the mantle rheology

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The region around core-mantle boundary is estimated to be composed of post-perovskite phase with some fractions of outer core material. It is unclear that how these two different materials interact with each other chemically and dynamically. To understand these interactions, it is important to know the effect of a metallic melt on the viscosity of silicate rocks.

According to Hirth & Kohlstedt (2003), strain rate is an exponential function of melt fraction \((d\varepsilon /dt \propto \exp(\alpha \phi))\) under a constant stress. With larger melt fraction, polycrystalline silicate becomes softer. Hustoft et al (2007) performed creep experiments on olivine+Fe-S and olivine+Au showing that the melt fraction factor \(\alpha\) is approximately one-fifth relative to the value of \(\alpha\) reported for olivine+MORB (Scott & Kohlstedt, 2006). However we don’t know how the rock viscosity is affected by a relative size of metallic melt against olivine grains and by strain. To understand these effects, we performed creep experiments on olivine+Au and compared the viscosity obtained from our experiments with the viscosity reported by Hustoft et al (2007).

We synthesized Fe-free olivine polycrystals with Au particles as follows; (i) We mixed fine powders of \(\text{Mg(OH)}_2\), \(\text{SiO}_2\), and Au. (ii) We made forsterite+enstatite from calcination of \(\text{Mg(OH)}_2\) and \(\text{SiO}_2\). (iii) We sintered the formed samples under a vacuum condition. Sintered materials contain forsterite, enstatite and Au with volume fractions of 81 %, 9 %, 10 %, respectively. Grain sizes of olivine and Au are 0.7 and 0.8 μm, respectively. We performed high-temperature and uniaxial compressional creep experiments on these materials at atmospheric pressure. We changed the stress from 10 MPa to 20 MPa, 40 MPa and 80 MPa at the constant temperatures (1200°C and 1300°C). Under each stress level, we measured a strain rate where the relationship between time and strain became linear (steady state creep). We observed microstructures of the aggregates after the experiments using scanning electron microscope (SEM).

Based on stress versus strain rate data, we obtained a relationship of \(d\varepsilon /dt \propto \sigma^{1.7}\). We observed that equiaxed Au particles became flattened against compressional direction after the experiments. The samples exhibited 4-8 times softer than Au-free samples which were synthesized by the same method we used. Our samples are even 3-4 times softer relative to the aggregates used in Hustoft.

In our experiments, Au particles deformed considerably, while the shape of the Au phases was not substantially changed at Hustoft’s experiments. We attributed this difference to relatively larger size of Au particles to olivine grains in our study compared to that in Hustoft’s sample. Substantial deformation of soft Au particles can increase the stress for olivine grains which enhanced creep rate.

Keywords: viscosity, metallic melt, olivine
Technical development and improvement for sound velocity measurements of liquid Fe-S up to 15 GPa using ultrasonic pulse-echo method

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Knowledge of the physical properties of liquid iron alloys is important for understanding the liquid core of the Earth and other terrestrial planets and satellites. Sound velocity is a key physical property to know the structure and composition of these cores because it can be directly compared with seismic observations. However, sound velocity measurements of liquid iron alloy by ultrasonic methods combined with multi anvil apparatus have been limited to below 8 GPa (Nishida et al. 2013; Jing et al. 2014; Kuwabara et al. 2016). Therefore, we have been developing and improving techniques that enable us to measure sound velocities of liquid iron alloys up to 20 GPa. Here we report newly established techniques for sound velocity measurements of liquid Fe-S up to 15 GPa.

High-pressure and high-temperature experiments were conducted at the AR-NE7A beamline at the KEK PF-AR synchrotron facility. High pressure was generated by Kawai-type multi anvil apparatus (MAX-III). High temperature was generated using cylindrical resistive heater made of Al₂O₃ + TiC composite. The sample was enclosed in a flat-bottomed cylinder container made of BN with a buffer-rod and a backing plate made of sapphire single crystal. We determined the pressure and temperature simultaneously without a thermocouple from the unit-cell volumes of NaCl and MgO by employing their equations of state. Sound velocity was measured by ultrasonic pulse-echo overlap method. The sample melting was identified during the experiments using X-ray diffraction, and was confirmed afterwards from textural observations of the run products. Preliminary results show the error in sound velocity of liquid Fe-S at 15 GPa is approximately 2.5% under good conditions. In our previous experiments, the error in sound velocity below 7 GPa was approximately 1% under the best conditions. Taking it into account, our newly techniques can provide satisfactory accuracy. Details and latest experimental results will be presented.

Keywords: core, sound velocity, liquid Fe-S, high pressure
Development for Neutrino Directional Measurement in Liquid Scintillator

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Liquid scintillator detector has a sensitivity to geo-neutrino. However, this detector can't observe direction of anti-neutrino. So we develop new-type detector that can know direction of anti-neutrino. In my poster, I talk about development of $^6$Li loaded liquid scintillator and high vertex resolution imaging detector.

Keywords: neutrino
High-pressure in situ X-ray laminography using diamond anvil cell

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The diamond anvil cell (DAC) is a powerful tool to reproduce high-pressure (P) and high-temperature (T) conditions, corresponding to those of the deep Earth interior, in a laboratory. Various types of measurements such as in situ high-P–T spectroscopic measurements and ex situ chemical analysis have been conducted using DACs to understand the structure and evolution of the Earth’s interior. Among these techniques, 3D visualization and textural/chemical characterization of the internal structure of samples at high-P–T is of great importance. Recently, the dihedral angle of molten iron between bridgmanite was investigated by imaging recovered DAC samples using X-ray computed tomography (CT), and the results provide important insights about the physical process of the Earth’s core-mantle separation (Shi et al., 2013). In situ high-P X-ray CT has been developed by transmitting X-rays through a light metal gasket, such as Be, between diamond anvils. To date, the applications have been limited to physical purposes, such as the changes of the volume or shape of the sample with pressure (Liu et al., 2008; Wang et al., 2012).

On the other hand, Tsuchiyama et al. (2013) developed a 3D chemical imaging technique, known as analytical dual energy microtomography, in which two X-ray energies below and above the absorption energy of a key element, such as Fe, are used for CT. We applied this technique to recovered DAC samples to determine the solidus temperature of pyrolitic mantle, using incompatible Fe enrichment as a signature of melting (Nomura et al., 2014). This dual energy technique has an additional advantage that artifacts in the reconstructed images, which are a typical problem in CT, can be avoided. The next step should be to carry out in situ high-P–T dual energy X-ray imaging, which remains challenging because deep Earth is composed of light elements (e.g. Fe, O, Si, Mg) with an X-ray absorption edge far below the hard X-ray energy range, in which the light metal gasket absorbs the incident X-rays crucially.

A high-pressure in situ X-ray laminography technique was developed using a newly designed, laterally open diamond anvil cell. A low X-ray beam of 8 keV energy was used, aiming at future application to dual energy X-ray chemical imaging techniques. The effects of the inclination angle and the imaging angle range were evaluated at ambient pressure using the apparatus. Sectional images of ruby ball samples were successfully reconstructed at high pressures, up to approximately 50 GPa. The high-pressure in situ X-ray laminography technique is expected to provide new insights into the deep Earth sciences.

Keywords: High pressure, X-ray imaging, diamond anvil cell
Development of resistance-heated diamond anvil cell using boron-doped diamond heater

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Laser-heated diamond anvil cell is the most successful method for reproducing the pressures and temperatures of the Earth's deep interior entirely in a laboratory (e.g. Tateno et al., 2010 Science). However, it is well known that laser-heating results in steep temperature gradients within a sample (e.g. Rainey et al., 2013). Such steep temperature gradients cause the solid-state chemical segregation called as ‘Soret diffusion’. This effect is well known in gas chemistry such that heavier elements or elements with larger ionic radii migrate from hot to cold regions, while the lighter elements move in the opposite direction (Grew and Ibbs, 1952). The Soret diffusion takes place not only in gas but also in liquid and solid. Therefore, Soret diffusion makes it difficult to perform chemical equilibrium experiments using laser-heated diamond anvil cell (Simmyo et al., 2008 JGR).

The technique for homogeneous heating has been developed, that is internally-heated diamond anvil cell. In this method, the heater is put into a sample chamber and compressed together with the sample. Because the diamond has a high thermal conductivity, diamond anvils do not become a high temperature and the heated zone is limited to near the sample chamber. Therefore, internally-heated diamond anvil cell has a potential to generate temperature more than 2000 K because the diamond anvils do not transform to the graphite. A sample was used also as a heater in previous studies (e.g. Liu and Bassett, 1975; Boehler et al., 1986). Therefore, only electric conductor can be used as a sample for the experiment. Zha and Bassett (2003) overcame this situation by making a small hole in a Re heater and filled the hole with sample. Both metal and nonmetal can be used as the sample in this method. The study showed that temperature gradients of Re heater near sample room were gentler than that of laser-heating studies. However, its temperature gradients were still steeper than multi-anvil’s temperature gradients (Canil, 1994).

On the other hand, the boron-doped semiconductor diamond heater is known to be able to have a much smaller temperature gradient than that of metallic heater (Yoneda et al., 2014). In multi-anvil experiments, Yoneda et al. (2014) successfully generate high temperature more than 3000 K, which Re and LaCrO₃ heaters cannot generate.

In this study, I developed the internally-heated diamond anvil cell technique using boron-doped diamond heater. The results showed that temperature gradients of boron-doped diamond heater in diamond anvil cell were smaller than that of metallic heater used in previous study (Zha and Bassett, 2003). In addition, its temperature gradients are as steep as multi-anvil’s temperature gradients. In this presentation, we will show our recent progress on this study.

Keywords: Diamond anvil cell, Boron-doped diamond, Internal resistive heating
Transportation of hydrogen by iron oxide-hydroxide in the Earth’s interior

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Water (hydrogen) plays important roles in dynamics in the Earth’s interior. It is expected that hydrogen is transported from the surface to the interior by the subducting slab. Hydrogen is also a candidate of the light element of outer core. Therefore, the study of the hydrogen in the Earth’s interior is quite important. Terasaki et al. (2012) investigated the reaction between Fe-Ni alloy and delta-AlOOH up to the pressure of core-mantle boundary. They showed that hydrogen is partitioned into Fe-Ni alloy and suggested that the core was hydrogenated by the subducting delta-AlOOH. Dobson and Brodholt (2005) proposed that the banded iron formation subducted to the core-mantle boundary and stagnated there. The banded iron formation contains iron oxide-hydroxide. Therefore, it is important to study the stability and properties of iron oxide-hydroxide under high pressures and high temperatures to discuss the transportation of hydrogen in the Earth’s interior. We carried out X-ray diffraction study and X-ray absorption measurement in the Photon Factory, Tsukuba, Japan. Goethite (alpha-FeOOH) is stable at ambient condition. However, it transformed to epsilon-FeOOH at 7.8+-0.5 GPa and 873K. Our previous study showed that epsilon-FeOOH was stable under the condition of the lower mantle. We suggest that epsilon-FeOOH can transport hydrogen to the core-mantle boundary and supply hydrogen to the outer core.

Keywords: hydrous phase, slab, mantle, banded iron formation, outer core
Possible link between East-west mantle geochemical hemispheres and Geoneutrino

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There has been an extensive debate concerning the compositional structure of the mantle: e.g., two-layered mantle model, stratified/zoned mantle model, plum-pudding mantle model, and marble-cake mantle model (e.g., Tackley, 2008; Iwamori, 2016, for review). The compositional structure is important as it reflects the flow pattern of mantle convection and differentiation processes during material cycling, yet poorly constrained at present. An geochemical end-member model argues that the mantle convection chaotically stirs geochemical heterogeneity brought by plate subduction, resulting in ubiquitously heterogeneous mantle (e.g., plum-pudding or marble-cake mantle, Zindler et al., 1984; Allègre and Turcotte, 1986). At the same time, a large-scale heterogeneity has been argued to exist, e.g., Dupal-anomaly in the southern hemisphere (Dupré and Allègre, 1983; Hart, 1984), or East-west geochemical hemispheres in terms of hydrophilic components (Iwamori and Nakamura, 2012; 2015).

Distributions and abundances of the radiogenic isotopes such as uranium (U) -238, -235 and thorium (Th) -232 in the mantle are key to constrain cooling history and mode of mantle convection of the Earth (e.g., McKenzie et al., 1974; Davies, 1999; Korenaga, 2013), because of the radiogenic heating. However, detailed information of distributions and abundances of such radiogenic elements in the Earth’s interior are not well constrained. Recently, Kamioka Liquid-Scintillator Antineutrino Detector measured the geoneutrino flux from decay of U-238 and Th-232. The observations indicate that the heat from radioactive isotopes might account for about a half of Earth’s total heat flux (The KamLAND Collaboration, 2011). In addition, Tanaka and Watanabe (2014) proposed Li-loaded directionally sensitive detector for possible geo-neutrinographic imaging. Based on these on-going measurements and new methods, the fundamental questions concerning the mantle compositional structures described above could be addressed.

East-west geochemical hemispheres of the mantle have been proposed based on statistical analysis (Independent Component Analysis) of the global isotopic data set of young basalts (Iwamori and Nakamura, 2012; 2015), suggesting that the eastern hemisphere is enriched in “anciently subducted fluid component”. If this is the case, we expect a systematic hemispherical difference in elemental abundances and ratios, including U and Th. Although the absolute abundances of these elements in the mantle are not readily constrained by the basalt data (unless the degrees of partial melting of basalts are tightly determined), by combining the geochemical analyses and geoneutrino measurements, we might be able to constrain the distribution and abundances of crucial elements, which will lead us to evaluate Geoneutrino.

Keywords: Mantle composition, Geoneutrino
Stability field of phase Egg under high temperature and high pressure: Possibility of phase Egg as a water reservoir in mantle transition zone

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Water in the earth’s interior is one of the main research topics because the water is known to affect physical properties of materials in the earth’s interior such as rheology, electric conductivity, seismic velocity, density, and melting point. The sedimentary layer of the oceanic crust transfers water into the deep earth mantle via subducting slabs (Peacock, 1990). Phase Egg, AlSiO3(OH), is one of the important hydrous phases in the mantle originating from the sedimentary layer and can contain H2O of 7.5 wt% as hydroxyl. However, two previous studies (Sano et al., 2004; Pamato et al., 2014) have reported different stability fields about phase Egg. This inconsistency leads to different earth-scientific outlooks on water cycling system via subducting slabs: whether the phase Egg can reserve water in the top of the lower mantle or not and where the superdeep diamond containing phase Egg originates (Wirth et al., 2007). Phase Egg as an inclusion in diamond might indicate a possibility that a top of the lower mantle might be wet.

Here, we conducted high-pressure experiments using Kawai-type 3000 ton multi-anvil apparatus and 1000 ton multi-anvil apparatus at Tohoku University in order to determine the stability field of phase Egg. Experiments were performed in the pressure range of approximately 17-21GPa and in the temperature range of 1000-1200℃. Starting material was a mixture of Al2O3, Al(OH)3, and SiO2 compounded similarly to ideal phase Egg composition, which was different from those of two previous studies (Sano et al., 2004; Pamato et al., 2014).

In this study, we found that phase Egg decomposed under the pressure corresponding to the mantle transition zone at 1000℃. This indicates that phase Egg is unstable in the top of lower mantle and can be a water reservoir in the mantle transition zone. In addition, this implies that the superdeep diamond, which Wirth et al. (2007) reported, does not originate from the lower mantle but from the wet mantle transition zone.

Keywords: water cycle in the earth’s interior, phase Egg, multi-anvil apparatus, high pressure and high temperature, mantle transition zone, superdeep diamond
Viscosity of basaltic magma at high pressure

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Viscosity and density control the mobility of magma. Sakamaki et al. (2013) measured the viscosity of basaltic magma at high pressure and reported the viscosity minimum around 4 GPa. They also measured the density of magma and found a quick elevation of the density around the pressure. On the basis of the results they proposed a model of stagnation of magma around the lithosphere-asthenosphere boundary (melt pond model). However, the pressure range of their measurement was limited to 7 GPa. Reid et al. (2003) carried out viscosity measurement of diopside melt to 13 GPa and reported the viscosity maximum around 10 GPa. They suggested that the decrease in viscosity above 10 GPa was caused by the structural change of melt. Therefore, the change in viscosity is also expected in basaltic magma. Here, we report the result of viscosity measurement of basaltic magma above 10 GPa. We adopted the falling sphere method using the X-ray radiography. Experiments were carried out at the beamline BL-04B1 in SPring-8. We found the decrease in viscosity between 7 and 10 GPa. Above 10 GPa the viscosity increased to 13 GPa. On the basis of the observation of seismic wave, the existence of melt around the base of the upper mantle (e.g., Revenaugh and Sipkin, 1994). We suggest the stagnation of melt by the change in viscosity.

Keywords: magma, viscosity, mantle
Thermal conductivity of lower mantle minerals from *ab initio* anharmonic lattice dynamics

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Determination of lattice thermal conductivity (\(\kappa\)) of lower mantle minerals is a key to understanding the dynamics of the Earth’s interior. Although determination of \(\kappa\) was impractical in the deep Earth \(P, T\) condition for a long time, recent experimental and computational developments have been extending the accessible \(P\) and \(T\) ranges (e.g. H. Dekura, T. Tsuchiya and J. Tsuchiya, Phys. Rev. Lett. 110, 025904, 2013). *Ab initio* prediction of \(\kappa\) requires understanding of the phonon-phonon interaction associated with the lattice anharmonicity. We recently succeeded in developing an efficient method to calculate it based on the density-functional perturbation theory combined with anharmonic lattice dynamics theory, and applying to MgSiO₃ perovskite in the whole lower mantle \(P, T\) range for the first time. Next we extend our techniques to other lower mantle minerals such as MgSiO₃ post-perovskite, and now calculations of more realistic Fe-bearing systems are also started. In this presentation, we introduce the current situation of our research on \(\kappa\).

Keywords: Earth’s lower mantle, Phonon transport property, First-principles calculation
Ab initio prediction of the incongruent melting relation in the MgO-SiO₂ system at multi-megabar

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Magnesium silicates are thought to be the major components of the mantle of terrestrial planets and the core of giant planets (Guillot, 1999; Seager et al., 2007). However, the thermodynamic phase equilibrium in the MgO-SiO₂ system is still not well studied at multi-megabar, including melting relations. A recent laser shock experience reported two discontinuous phase changes in MgSiO₃ at 300-400 GPa (Spaulding et al., 2012), but an ab initio molecular dynamics study identified no clear transition in MgSiO₃ liquid (Militzer, 2013). Boates and Bonev (2013), on the other hand, examined a decomposition reaction of liquid MgSiO₃ into solid MgO and liquid SiO₂ and reported that liquid MgSiO₃ is dissociated at ~300 GPa. This result implies a possible incongruent melting. However, the reaction they considered is too simple and unrealistic. The detailed phase diagram in the MgO-SiO₂ system is therefore required to be clarified at multi-megabar. In this study, we perform ab initio free energy calculations based on the thermodynamic integration method (Kirkwood, 1935) and determine the melting phase relation in this binary system.

Keywords: ab initio calculation, MgO-SiO₂ system, incongruent melting, multi-megabar
Geoelectromagnetic jerks produced by heterogeneous electrical conductivity in the D'' layer

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Geomagnetic jerks are identified at 2003, 2007 and 2011 in the Atlantic and Indian Ocean. It has been suggested by Chulliat et al. (2015) that the regional nature of the geomagnetic jerks and spatio-temporal variations of geomagnetic secular acceleration can be explained by fast equatorial magnetohydrodynamic waves propagating near the surface of the Earth’s core. On the other hand, the geoelectric field observed using long baseline submarine cables in the northwestern Pacific also showed sudden change of its secular variation at 2006. In a previous study, we showed using a simplified mantle conductivity models that the geoelectric field variation and the geomagnetic jerk in 2007 can have the same origin; the variations can be generated by a sudden change of the toroidal magnetic field secular variation in the core and influence of high electrical conductivity region in the D'' layer beneath the area where the geomagnetic field variation was evident. Since the geoelectric and geomagnetic field variations can have the same origin, we call the variations a geoelectromagnetic jerk. In this presentation, we show results of numerical experiment on the electromagnetic field in the mantle due to the toroidal magnetic field variation in the core employing more realistic distribution of the electrical conductivity in the D'' layer based on the SH-wave velocity model obtained by Takeuchi (2012). Conductivity heterogeneity at the Earth’s surface due to the conductivity contrast between the land and seawater on the electric field is also included in the numerical experiment to examine its effect on the voltages observed by submarine cables. Typical spatio-temporal variations of the observed and simulated geoelectromagnetic field are examined to consider plausibility of geoelectromagnetic jerk hypothesis.

Experimental and theoretical thermal equations of state of MgSiO$_3$ post-perovskite at multi-megabar pressures

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The MgSiO$_3$ post-perovskite phase is the most abundant silicate phase in a super-Earth’s mantle, although it only exists within the Earth’s lowermost mantle. We established the thermal equations of state (EoS) of the MgSiO$_3$ post-perovskite phase, which were determined by using both laser-heated diamond anvil cell (LHDAC) and density-functional theoretical techniques, within a multi-megabar pressure range, corresponding to the conditions of a super-Earth’s mantle. The LHDAC experiments were performed at up to a pressure of 265 GPa at a temperature of 300 K, and 170 GPa at 2560 K. The ab initio calculations were performed at up to 1.2 TPa and 5000 K. The Keane and AP2 EoS models, which include parameters that limit to infinity at high pressure, were adopted for the first time to extract meaningful physical properties. The experimental volume data in a wide pressure-temperature range enabled us to determine the fully experimentally based parameters for the Mie-Grüneisen-Debye model. The Grüneisen parameter and its volume dependency were found to be consistent with their theoretically obtained values. Both the experimental and theoretical EoS are also found to be in very good agreement with one another, within 0.1% in volume at the earth’s core-mantle boundary condition, and the relation is maintained within 0.8% even up to a pressure and temperature of 300 GPa and 5000 K, respectively. Our newly developed EoS should be applicable to a super-Earth’s mantle, as well as the Earth’s core-mantle boundary region.

Keywords: post-perovskite, equation of state, super-Earth
Sensitivity of Core Phases on F-layer

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Last year we showed that the dispersion in PKPbc and differential traveltimes between PKiKP and PKPbc are particularly sensitive to the F-layer structure (lowermost outer core) and are insensitive to the structure of the other parts of the Earth (Ohtaki and Kaneshima, 2015). In previous studies, the Vp structure of the F-layer have been investigated using absolute traveltimes of PKPbc/c-diff, differential traveltimes between PKPbc/c-diff and PKIKP, amplitude ratios between PKPbc/c-diff and PKIKP, and the position of the C-cusp. PKIKP pierces the inner-core boundary and turns in the inner core; PKPbc turns in the lower part of the outer core; PKPc-diff diffracts on the inner-core boundary beyond the C-cusp; PKiKP reflects on the inner core boundary.

In this study we discuss the sensitivity of various core phases (PKIKP, PKPbc, PKPc-diff, and PKiKP) to the F-layer structure in detail. Among these observations, absolute traveltimes of PKPbc are affected by crustal and mantle structures that are strongly heterogeneous and are not precisely known, which indicates benefits of analyzing differential travels times. Differential traveltimes suppress the effects of heterogeneous structures as well as the discrepancy between a reference seismic model and the real Earth above the turning depths of rays. However, it is difficult to discriminate the P-wave velocity of the F-layer from that of the inner core using the differential traveltimes between PKPbc/c-diff and PKIKP, because the inner core is more heterogeneous than the F-layer. Fine structure of the F-layer is also poorly constrained by the amplitude ratios because of the low sensitivity of the ratios to the Vp gradient and of a trade-off between the Vp profile of the F-layer and the attenuation values in the inner core. The C-cusp position can be constrained only poorly by the amplitude observations, and there exist many velocity profiles that yield the same C-cusp position. In summary, conventional observations are obviously insufficient to resolve detailed F-layer structure.

In our previous study (Ohtaki et al., 2012), we examined the seismic structure near the inner core boundary beneath the South Pole. In that study, we investigated the velocity above the inner core boundary using the amplitude ratios between PKIKP and PKPbc/c-diff, assuming a constant velocity in the F-layer, because the ratio is not so sensitive to the velocity gradient, as mentioned above. In this study, we also examine a tolerance level of a velocity gradient there.

Keywords: Seismic velocity, Outer Core
Anomalously large PKiKP/PcP amplitude ratios at frequency of around 1 Hz observed by USArray

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Tanaka and Tkalcic (2015) observed the frequency dependent PKiKP/PcP amplitude ratios by Hi-net, of which ray paths are passing below the Western Pacific. They showed the existence of a spectral peak at approximately 2 to 3 Hz, a spectral hole at 1 and 3 Hz, and no peak and hole, suggesting lateral variations at the inner core surface. Here I report frequency dependent PKiKP/PcP amplitude ratios observed by USArray, of which reflection points are located below the Central America. I find also a large scatter of the frequency characteristics. Interestingly, the spectral peaks in the PKiKP/PcP spectral ratios around 1-1.5 Hz are detected when the reflection points are located below the east of Mexico that is not observed by Hi-net. The peak amplitude is about 2 times greater than that around 2 Hz. Based on the finite difference simulations by Tanaka and Tkalcic (2015), this observed peak can be explained by ICB sinusoidal topography with wavelength and height of 0.5 km, or ICB spiky topography with wavelength and height of 1.5 km. This observation suggests that the crystallization at the inner core surface or inner core growth system below the east of Mexico is different from that below the Western Pacific.

Keywords: Inner core, USArray, PKiKP/PcP
On the possible scenario of thermal evolution of Earth’s core with high thermal conductivity in a coupled core-mantle evolution model

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The thermal conductivity measurement of iron alloy from high P-T physics suggested to range from 60 to 150 W/m/K under temperature and pressure condition in Earth’s core [e.g. Gomi et al., 2013]. The previous study by Nakagawa and Tackley [2015] indicated that the CMB heat flow was just only 6 TW and, as a result, the magnetic evolution would be failed with high thermal conductivity and colder CMB temperature (~3500 K) caused by large adiabatic temperature gradient across the Earth’s core (~1 K/km) [Labrosse, 2015]. Here we assume smaller adiabatic temperature gradient across the Earth’s core (0.5 to 0.7 K/km taken from lower-bound value in Ichikara et al. [2014]) as well as high thermal conductivity of Earth’s core set as 120 W/m/K. For the successful scenario of a coupled core-mantle thermal evolution matching the current size of the inner core and continuous magnetic field generation, the CMB heat flow at the present time-scale would be around 12 TW because the CMB temperature is still high (~4000 K) for finding the current size of the inner core and the age of the inner core would be 1.2 billion year, which seems to be a bit older age of inner core compared to other studies [Labrosse, 2015; Davis, 2015]. To find the successful scenario of thermal evolution of Earth’s core, the adiabatic temperature gradient across the Earth’s core prescribed by Grueneisen parameter and bulk modulus would be quite important in terms of high CMB heat flow than could find the continuous magnetic evolution under the high thermal conductivity. With the lastest update of core-mantle evolution, the adiabatic temperature across Earth’s core would be consistent with the range found from first principle calculation rather than that used in the core evolution models approximated heat transfer across the CMB.

Keywords: Earth's core, Heat flow across the core-mantle boundary, Adiabatic temperature gradient, Thermal conductivity