Development of nano-polycrystalline diamond anvil cells for neutron diffraction experiments under high-pressure

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Neutron diffraction requires significantly larger sample volume than the case of x-ray diffraction because of the relatively small scattering cross section, so that crystallographic studies by neutron diffraction have long been limited to 30 GPa by using the Paris-Edinburgh press (Klotz, 2012), which enables to load larger volume of samples than conventional diamond anvil cells (DACs). Recently, conically shaped single crystal diamond anvils were applied for high-P neutron diffraction for ice VII, and the highest pressure record of 94 GPa was established by Boehler et al. (2013). On the other hand, we have noted that nano-polycrystalline diamond (NPD) rather than single crystal diamond could have a great potential for neutron diffraction (e.g., Okuchi et al., 2010), because of its orientaion-independent hardness owing to the absence of cleavage. Here we report on the development of originally designed anvil cells by using NPD specifically for neutron diffraction studies. Cylinders of NPD with 6 mm diameter and 6 mm height were supplied from GRC, Ehime Univ. and cut and polished to single beveled anvils with 1 mm culet diameter by Syntek co., ltd. Stainless steel (SUS301) drilled with 0.5 mm hole were used as gaskets. Load was applied by the Paris-Edinburgh press (VX2), which was placed on the gonio stage of the beamline PLANET (BL11) in J-PARC. We managed to obtain neutron diffraction from iron oxide up to at least 40 GPa without any damage of anvils, but the diffraction peaks were broadened when deuterated glycerol was used as pressure transmitting medium. We are now developing a gas-loadable cell and it will be tested near future.

Keywords: Neutron diffraction, Technical development, Nano-polycrystalline diamond

Development of rotational diamond anvil cell for deformation experiments under ultra-high pressure corresponding to Earth's core

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Development of high-pressure (static compression) experiments enabled to increase pressure up to ~360 GPa, corresponding conditions to inner core of the Earth (e.g., Tateno et al., 2010). On the other hand, pressure is limited for a technical reason in high-pressure deformation experiments. Earth’s interior is dominated by ‘dynamic’ processes. Therefore, expansion of pressure range in deformation experiments is necessary to understanding the evolution of Earth’s deep interior. We developed rotational diamond anvil cell (R-DAC) to conduct deformation experiments with large strain under ultra-high pressure conditions, corresponding to those of Earth’s core.

In this study, existing diamond anvil cell (DAC) is modified to give torsional deformation to sample under ultra-high pressure conditions. In the developed R-DAC, lower anvil is fixed and upper anvil can rotate to relative to the lower anvil. We deformed periclase (one phase), and mixture of bridgmanite and ferropericlase to test this apparatus. The experimental conditions are ranging 35–150 GPa, room temperature and strain-rate of 5.6×10^{-5}–1.7×10^{-4} s^{-1}. Starting material was grooved by FIB and the groove was deposited by Pt as strain-marker. Recovered samples were cut by FIB to observe the rotation angle of strain-marker, sample thickness, and shape of strain-marker in each cross-section. Deformation experiments were conducted also in Japan Synchrotron Radiation Research Institute (SPring-8) and 3D visualization of the internal structure of samples were performed using X-ray laminography (Nomura and Uesugi, 2016).

The geometry of strain-marker in recovered samples show nearly simple shear, indicating that this apparatus allows us to investigate the deformation with large strain under ultra-high pressure conditions, corresponding to those of core-mantle boundary (CMB). The rotation angle of strain-marker in recovered samples were compared to that expected from rotation angle of upper anvil. The results indicated that slip occurred between upper anvil and samples. Therefore, the combination of R-DAC and X-ray laminography, which can perform in-situ 3D observation of strain marker, is a valid and feasible way.

Recovered sample was observed using FE-SEM. Microstructure of mixture of bridgmanite and ferropericlase showed that ferropericlase highly deformed and connected each other. Although this prototype of R-DAC has some points that should be improved, we present preliminary results and potential of R-DAC to conduct ultra-high pressure deformation experiments.

Keywords: Deformation experiment, Diamond anvil cell (DAC), Lower mantle, Core

In situ 3D textural observations at high pressure and high temperature using X-ray laminography technique in diamond anvil cell

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High-pressure and -temperature experiments have been widely conducted using diamond anvil cells to understand the structure and evolution of the Earth’ s interior. Nowadays, 3D visualization technique has been developed to observe internal structure of the sample recovered from high pressures (Shi et al., 2013; Nomura et al., 2014). In addition, *in situ* high-pressure X-ray computed tomography techniques have been developed by transmitting X-rays through a light metal gasket such as Be (Liu et al., 2008; Wang et al., 2012). Using these techniques, geometric information such as the changes of the volume or shape of the sample with pressure is obtained. However, it is difficult to generate high-pressure and -temperature of the Earth’ s lowermost mantle or the core with keeping sufficient sample thickness when light metal is used as a gasket.

To overcome this problem, Nomura and Uesugi (2016) introduced X-ray laminography technique (Gondrom et al., 1999) to diamond anvil cell. In X-ray laminography, the rotational axis of the sample is inclined to the direction of the incident X-ray beam. Therefore, the incident X-ray beam can avoid the metal gasket surrounding the sample; it is no longer necessary to use a light metal as a gasket. However, it is still challenging to combine such measurements with heating technique in the diamond anvil cell.

Here, to carry out *in situ* high pressure and “high temperature” X-ray imaging, we have introduced the internally resistive heating method by using boron-doped diamond as a heater material. Boron-doped diamond has high X-ray transmissivity and can generate high temperatures more than 3000 K with high stability (Yamada et al.,2008; Shatskiy et al., 2009; Yoneda et al., 2014; Xie et al., 2016). We performed X-ray laminography experiments at BL47XU, SPring-8. The sample was Au foil, heater was boron-doped diamond and pressure medium and heat insulator was Al_2O_3. We have obtained the X-ray transmission images of the sample at 20 GPa during heating. Obtained images were sufficiently clear, despite of the Re gasket and boron-doped diamond heater surrounding the sample. We have reconstructed cross-section images of the sample before and after heating. These cross-section images showed that the shape of the sample was largely altered by heating due to melting. The technique developed in this study will provide new method to determine the melting temperature of the sample at high pressure. Our current results demonstrate that the X-ray laminography can be a powerful tool for understanding dynamic process in the deep Earth’ s interior, such as melting of the terrestrial materials.

Keywords: Diamond Anvil Cell, X-ray Laminography, In situ 3D textural observations

Evaluation of the pressures measured in the double stage diamond anvil cell technique

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The double stage diamond anvil cell (dsDAC) is claimed as an advance technique to generate a TPa static pressure (Dubrovinskaia et al. 2016). Although the nanocrystalline diamond semi-balls were used for the TPa generation, it is need to prepare an desired anvil shape; i.e., the culet and bevel size and so on, in order to control the pressure distribution at the tip of the 2nd anvils. We have been trying to develop the dsDAC as a well-controlled experiment device using the focused ion beam (FIB) system (Sakai et al. 2015).

Here we report the results of the dsDAC experiments using the newly synthesized nanopolycrystalline diamond (NPD) with a single-nano grain size as a micro-anvils material. The 2nd stage micro-anvils are shaped with 3 um culet and 10 um bevel using FIB system (Scios, FEI). The tiny rhenium disc (3 um diameter and 1 um thickness) was used as a sample. The other experimental procedure was generally same as in Sakai et al. (2015). The X-ray diffraction (XRD) experiments were performed at SPring-8 BL10XU in order to determine the generated pressure from the lattice parameter of rhenium. The diffraction patterns from the rhenium sample showed very broad peaks due to the large pressure gradient at the tip of the micro-anvils as contrasted with the sharp peaks observed in previous works (Dubrovinsky et al. 2012, 2015; Dubrovinskaia et al. 2016). The deconvolution of the peak results that the rhenium was compressed to be $V/V_0 = 0.633$. According to the equation of state of rhenium (Re-EoS) reported by Anzellini et al. (2014), it corresponds to about 430 GPa. On the other hand, it is 630 GPa if we adapt the Re-EoS by Dubrovinsky et al. (2012). In the term of V/V_0 value, we reproduced the result of Dubrovinsky et al. (2012) although we observed the X-ray diffraction peaks with large FWHM as an unavoidable result from the large pressure gradient at the tip of the 2nd stage micro-anvils.

The compression behavior of NPD micro anvils shows a monotonous volume decrease along the equation of state of the diamond (Dewaele et al. 2008); however it becomes incompressible when the compression by the 2nd stage micro-anvils started. It is a well-known phenomenon induced by the uniaxial stress, i.e., the overestimation of the volume. This large effect of uniaxial stress was released when the 2nd stage micro-anvils failed, which means the sudden volume decrease occurred although the pressure was dropped. This “incompressible” feature is the opposite of the “compressible” behavior which reported in Dubrovinsky et al. (2012).

The dsDAC certainly has a potential ability to generate an ultra-high pressure. Since the X-ray beam is comparable in size to the culet of the 2nd stage micro-anvils, it needs further evaluation of the relationships between the X-ray beam intensity profile and the pressure distribution and the sample distribution to interpret the XRD patterns measured in the dsDAC experiments correctly.

Keywords: Double stage diamond anvil cell (dsDAC), Nanopolycrystalline diamond (NPD), Tera Pascal (TPa), Focused ion beam (FIB) system, Equation of state (EoS)

Generation of ˜90 GPa in Kawai-type multianvil apparatus using nano-polycrystalline diamond anvils.

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Nano-polycrystalline diamond (NPD) has higher hardness, toughness, elastic stiffness, and X-ray and light transmittance than conventional sintered diamond (SD). These properties make it suitable for use as an anvil material in high-pressure experiments. Kawai-type multi-anvil apparatus (KMA) has been widely used in high-pressure experiments, where accurately controlled pressure and temperature in larger sample volumes relative to diamond anvil cell are available using tungsten carbide (WC) or SD as the second-stage anvil materials. However, the generated pressures in KMA with these conventional anvils at high temperatures have been limited to about 40 GPa and 100 GPa, respectively, by using these materials as the anvils. We have been attempting to generate further higher pressures using NPD cubes with the "6-6-8" anvil configurations. *In situ* X-ray diffraction measurements and radiographic imaging observations were performed at the large-volume press beamline, BL04B1, SPring-8. Baked pyrophyllite gasket and semi-sintered Al_2O_3 pressure medium were used, and a folded gold foil was placed in the center of the pressure medium as a pressure marker. The maximum pressure so far achieved at room temperature is about 88 GPa at a press load of 3.4 MN, which is far higher than that achieved using SD anvils (˜56 GPa) with the identical cell assembly and the press load. Moreover, it was found that both in situ X-ray diffraction measurements and imaging observations are possible even through the NPD anvils, which is great advantage over the experiments using SD anvils where the invisibility of the sample becomes a serious issue due to the plastic deformation of anvils under such high pressure. Thus, we conclude NPD is highly promising anvil material for the next generation KMA technology.

Pressure generation of 120 GPa and stability of bridgemanite

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Physical and chemical properties and structure of materials are strongly depend on the pressure and temperature. $MgSiO_3$ bridgemanite, which is the most abundant mineral in the lower mantle, undergoes the phase transition to post-perovskite structure ($CaIrO_3$, Cmcm) at pressure and temperature corresponding to the D” layer conditions, discovered by diamond anvil cell high pressure experiments (Murakami et al., 2004). This phase transition is considered to a key to understand the mantle dynamics and therefore precise determination of the phase boundary is important, for example, effect of the other elements (e.g., Fe, Al and Fe^{2+}/Fe^{3+}). In this study, we developed the high pressure generation technique in a Kawai-type multianvil apparatus, which enables us to obtain large volume sample (~0.1 mm^3) with stable heating and homogeneous high temperature distribution in the sample, and tried to determine the phase boundary between bridgemanite and post-perovskite.

We conducted pressure generation test by using a Kawai-type large volume press (SPEED mk.II) at SPring-8 synchrotron facility. For the cell assembly, we used Cr-doped MgO as pressure medium, $BN+TiB_2$ as heater because of high transparency for X-ray and soft fired pyrophyllite as gasket. Temperature was monitored by $W_{97\%}Re_{3\%}$-$W_{75\%}Re_{25\%}$ thermocouple whose junction was located in the heater. Before experiment, we prepared the sintered starting material of the mixture of $Mg_{0.9}Fe_{0.1}SiO_3$+5wt % Al_2O_3 bridgemanite and gold which was used as the standard to estimate the pressure (Tsuchiya, 2003) in the ration of 1/6 in weight. During compression in the experiments, we frequently pre-heated the sample to 800-1100 K at every 5-10 GPa for the relaxation of stress stored in the cell assembly to reduce the probability of “blow out”.

We finally succeeded to generate pressure to 120 GPa with press load of 13 MN at an ambient temperature after pre-heating at 800K. Then we again heated up sample to 1673 K to observe the phase transition from bridgemanite to post-perovskite at 105 GPa because a large pressure drop occurred down to 105 GPa at higher temperature than 800 K during heating up. The obtained diffraction pattern was completely indexed as bridgemanite, indicating the stability field of bridgemanite with the composition of $Mg_{0.9}Fe_{0.1}SiO_3$+5wt % Al_2O_3. The present result is consistent with previous study in $MgSiO_3$ (Tateno et. al., 2009). They reported the phase boundary to be 110 GPa at ~1673 K. As a conclusion, the effect of 10 mol % of iron component and 5 wt % of Al_2O_3 is less than 5 GPa on phase boundary shift in pressure.

3D reconstruction of light emission points for geo-neutrino directional measurement

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Observation of geo-neutrinos is a new and unique way to observe Earth's interior directly. Geo-neutrinos are anti-electron neutrinos emitted by beta-decays of radioactive elements such as Uranium, Thorium and Potassium. They tell us some information of chemical composition of the Earth's interior and heat source distribution. The KamLAND experiment led by Tohoku University succeeded in observation of Geo neutrino for the first time in the world and constrained on Earth models.

Liquid scintillator detectors have sensitivity to low energy neutrinos such as geo-neutrinos, but on the other hand they can't measure neutrino directions. Therefore we started to develop directional sensitive liquid scintillator detector. We are planning to measure directions of neutrinos by using Li loaded liquid scintillator and imaging cameras which can detect light emission points precisely. Neutrino directional measurement will bring us new tool to distinguish crust and mantle contributions and to remove reactor neutrino background.

To obtain information of neutrino's directions, it is necessary to precisely measure positions of prompt positron signal and delayed neutron capture signals. In previous studies, we demonstrated to be able to measure reaction points caused by gamma-ray from radiation source with an imaging camera. The goal of this study is 3D reconstruction of neutron's light emission positions by two imaging cameras. I will explain a present state of our study which aims to establish new techniques for neutrino directional measurement.

Keywords: geo-neutrino, neutrino directional measurement

Lithology Distribution Model for Neutrino Flux Simulations Obtained by Using Bayesian Inference

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It is well-known that geo-neutrino observations provide critical constraints on the mantle chemistry. Because chemistry (i.e., distribution of U and Th concentration) in the local crust also affects to the neutrino flux at the detector, it is widely recognized that developing local chemistry model is one of the most important steps in the geo-neutrino simulations. In previous studies, they used various geological insights to obtain the chemistry models, however, in most cases, the modeling is not well tractable, and the uncertainties of the obtained models are not very clear. Because our final goal is to obtain the probability density function of the neutrino flux at the detector, we need more quantitative and reproducible approach.

In this study, we propose Bayesian approach to obtain the statistical chemistry model. To do this, we adopted two-step approach; we fist obtain statistical lithology distribution model and then combine it with the statistical concentration model for each lithology type that is presented by Ueki (2017, this meeting). In this presentation, we focus on the method and results of the first step.

The lithology model in this study consists of probability of the lithology type at each point in the local crust. It is definitely different from the previous models that definitely state the lithology type. To obtain this probability, we use the Bayesian theorem. We first define some a priori probability and then modify it using observational and experimental information. To take the regional specialty of Japanese crust into account, we assume the bulk composition of the Hidaka metamorphic belt as the a priori probability. To modify it, we use the information of the P wave tomography model by Matsubara et al. (2008), laboratory measurements of P-velocity of each lithology by Christensen and Mooney (1995), and the temperature structure model by Furukawa (1995). The detailed method and results will be shown in the presentation.

Keywords: neutrino, lithology, tomography

U, Th concentrations of Japanese rocks for geo-neutrino modeling

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With the aim of determining the amount of radioactive elements contained in the earth's core and mantle with high precision, using the world's highest precision earth neutrino data obtained with KamLAND, we are conducting lithological modeling of the crust of the Japan arc using the seismic velocity structure data.
In order to estimate the uranium-thorium concentration of the Japanese Island Arc crust using the result of the lithological distribution obtained from the seismic velocity structure, We constructed the database of the chemical composition, especially the uranium and thorium concentrations and some major elements of the rocks of the Japanese arc. It consists of data of more than 10000 points, data of about 100 papers and reports. In addition, we carried out the sampling and chemical analysis of the lower crustal xenolith from Japan arc.
By using the uranium-thorium concentration of various rocks of the Japanese arc, it is possible to estimate the uranium-thorium concentration in the Japanese arc, and thus to more realistically estimate the neutrino flux from the crust is possible.
Variations of U-Th concentrations can be explained by the melt process such as melting and crystal differentiation, U enrichment due to alteration at the ocean floor, U loss at the ground surface. In addition, the average value of the composition was somewhat depleted than the estimation using the continental crust.
Using the compiled compositional data, we model the probability distribution to calculate chemical composition distribution and neutrino flux. Although in the previous geochemical studies, log-normal distribution or gaussian distribution has been widely used, the gamma distribution is newly used in this study. In addition to numerous advantages in mathematical usages, it also has the advantage of being able to adapt to both symmetric and asymmetric distributions, do not have negative values, and it can accurately reproduce the sample mean. In addition, the gamma distribution has been used to model the chemical processes such as protein concentration.
By using the probability density function for each rock type which is represented by the gamma distribution, it enables us to estimate the compositional distribution of the arc crust of the Japanese arc and thus the more realistic neutrino flux from the crust.

Keywords: Arc crust, Geo neutrino, radiogenic elements

Current Status of Development for Geo-Neutrino Directional Measurement

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Neutrino is one of the elementary particle and neutrino physics has been developing. Liquid scintillator (LS) detectors have a good sensitivity to low energy anti-neutrinos. However, unlike water Cherenkov detectors, LS detectors are not sensitive to anti-neutrino direction. Directional sensitive LS detector has possibility that it can reveal information. For example, it will contribute to better understanding of the Earth’ s interior using geo-neutrino flux measurement in kton scale detector, and there is possibility of application to reactor monitoring system in small size detector.
Anti-neutrinos are detected by inverse beta decay reaction and tagged by the delayed coincidence method (prompt signal is positron and delayed signal is neutron capture event) that provides a powerful tool to suppress backgrounds. Although the emitted neutron retains the directional information of incoming anti-neutrinos, current LS cannot identify neutron capture point before directional information is lost. Li-loaded LS has the ability to shorten the neutron capture range because of large neutron capture cross section (940barn cf. ^{1}H 0.3 barn) of ^{6}Li and neutron capture point is point-like because alpha ray and ^{3}H are emitted after neutron is captured by ^{6}Li.So we can know directional information of anti-neutrino by observing positron reaction point and neutron capture point.
And, to separate prompt and delayed points clearly, optical discrimination of energy deposit points by high resolution imaging devices is also required. We are planning to use reflective optical system and multi-channel photomultiplier as an imaging device. Recently, we were able to image ^{6}Li capture event.
I will report about the current status of development for geo-neutrino directional measurement.

Keywords: neutrino, Liquid scintillator

Geoneutrino Flux Estimation based on Probabilistic Lithology and Compositional Models

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Geoneutrino observation with the KamLAND detector at Kamioka, Gifu, is expected to bring unique knowledge on the interior of the earth. However, due to a large contribution of the nearby crust to the total geoneutrino flux at Kamioka, detailed understanding of the Uranium and Thorium distributions in Japanese crust is crucial. For this purpose, we have been developing a lithology model by seismic tomography, rock composition models based on evaluated vast samples, and a method to properly propagate all the probabilistic information to an estimation of the geoneutrino flux at Kamioka.

Geoneutrino observations are statistical, therefore results from the observations, such as the total heat budget in the mantle, are described with probability distributions. In order to properly do this, the nearby crustal model must be described in the language of probabilities, where estimation of uncertainties, not just the central value, has essential importance. In spite of this, no geoneutrino flux model with objective uncertainty estimation has never been constructed, presumably due to lack of input information and methodological difficulty of doing it.

At this presentation our effort on developing the method of estimating the geoneutrino flux based on probabilistic input models will be discussed. Currently our major difficulty is description and evaluation of correlations among values in the input models, such as quantitative description of regional lithological similarities and modeling of compositional variations / similarities among rocks classified as same rock type. In parallel to the effort of constructing the best optimal models, we evaluated a conservative uncertainty by assuming the maximum correlations among everything.

Although the estimated conservative uncertainty, 60~70%, is too large to be meaningful in geophysics, this is the first objective estimation of the uncertainty on the regional geoneutrino flux. We will also discuss the future prospects to further improve the estimation. In addition, some other interesting side-products, such as a heat-source distribution map of the 3-D Japan crust, will be presented.

Keywords: geoneutrino, BSE, thermal evolution, crustal composition

A review of thermal state of the shallow part of the Earth’s lithosphere: What we know and do not yet know

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To improve our understanding of the thermal evolution and structure of the deep Earth, it is necessary to know the shallow part of them. Surface heat flow provides important constraint on in. However, the number of heat flow data is limited and spatially very inhomogeneous and even in regions with measurements the data quality varies. To provide an attempt at a higher resolution map of heat flow, thermal conductivities are measured using sampled cores and used from existing and newly collected data. Also, to estimate the heat flow using geothermal gradient data, the closest thermal conductivity data is used for each gradient data. This approach does not take into account geological and hydrodynamical models to use the thermal conductivity, but this assumption works well enough to provide rough estimates of heat flow from geothermal gradient.

Meanwhile, there exist many indicators that are proxies for quantifying the thermal structure. One of the promising indicators is the cut-off depth of shallow seismicity. Several studies have been conducted to assess the inverse correlation between the cut-off depth and heat flow, since it has attributed primarily to the temperature. Another indicator is the depth of magnetic sources based on spectrum analysis of magnetic anomaly data. This analysis is still controversial, however, good correlation between estimated depths of crustal magnetic sources and heat flow suggests that this depth may reflect the broad average temperature. We address the advantages and limitations of each data and method.

Keywords: heat flow, thermal conductivity, seismogenic layer thickness

High precision analysis of W isotopes for OIB and MORB samples

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^{182}W is a decay product of ^{182}Hf ($t_{1/2}$=890 million year) which is extinct at now. The amount of ^{182}W can give information on evolution of very early solar system at the timescale from several million years from the solar system initial. Hf and W is a highly refractory element and the ^{182}W isotope evolution process in the bulk Earth could be the same as in chondrites. However, W is a highly siderophile element and Hf is a lithophile element. These elements could be partitioned into metal (core) and silicate (mantle) phases, which leads to higher Hf/W ratio of mantle.

To elucidate the core-mantle evolution of the early Earth, we have developed the high precision W isotope analysis using MC-ICP-MS (Thermo co. Ltd. NEPTUNE Plus) and have applied it to some OIB and MORB samples, such as Hawaiian basalts, South Africa Kimberite, Ontong Java Plateau lavas and Indian MORB.

We will present the W isotopic composition obtained for these samples and will discuss the early core-mantle co-evolution and core-mantle interaction, based on the W isotope, Os isotopes.

Keywords: Core-Mantle co-evolution, Tungsten isotope ratio, Hf-W system

Micro-volume stable isotope measurement using IRMS and its application in high pressure research

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Sulfur, oxygen, hydrogen and carbon are potential light elements candidates that might be present in the core in significant quantities to counter the density deficit of the metallic core. Based on geophysical consideration and high-pressure experiments, the core composition and its evolution have been focus of several previous studies. However, recent studies have predicted that there is a possibility of isotope fractionation at high temperature and high pressure conditions, especially in the magma ocean environment and core segregation (e.g. Satish-Kumar et al., 2011; Labidi et al., 2016). In order to understand the light element isotope fractionation processes in the deep earth it is necessary to measure isotope composition accurately in micro to nano scales from high pressure experimental run products.
At Niigata University, MAT-253 mass spectrometer (Thermo Fisher Science) was installed by the MEXT Grant-in-Aid for Scientific Research on Innovative Areas. The carbon and oxygen is measured using CO_2 and sulfur stable isotope measurement is carried out using SF_6 gas. We have completed the construction of vacuum inlet line for standard and sample gas, and evaluated the precision of carbon and oxygen isotope using CO_2 and for sulfur using SF_6 using the normal bellows sample reservoir. A new micro-volume inlet system was also installed and fundamental parameters such as pressure effect and capillary effect relating to micro-volume inlet system were tested. In the measurement using CO_2, standard gas in normal bellow showed a drift in both of carbon and oxygen isotopes were observed for six hours of continuous measurements ($\delta^{13}C$ = -0.172 ‰, $\delta^{18}O$ = -0.366 ‰) Therefore, we increased the volume of standard gas and obtained a better precession for the same sample duration. Internal carbon isotope standard sample of graphite (SP1 graphite powder), gave a precession of 0.045 ‰(n = 10). In the poster, we also present the details of the newly-constructed SF_6 gas preparation using curie point pyrolizer and gas purification system using gas chromatography. A new method for micro sampling using a femto-second laser ablation is also being tested for the analysis of small volume samples obtained using high-pressure experiments.

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Keywords: Sulfur isotope, Carbon and oxygen isotopes, Mass spectrometer

Metasomatic mobilization of PGE in the suboceanic mantle: an implication from sub-μm-sized sulfides from Tahitian peridotite xenolith

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Platinum-group elements (PGEs: Os, Ir, Ru, Rh, Pt and Pd) are strongly partitioned into metallic phases. Hence PGEs are thought to have been mostly sequestered in Earth's core during core–mantle differentiation. In spite of such preferential distribution of PGEs into the core, investigations of natural mantle peridotites have revealed that PGE concentrations of the mantle are enriched, i.e. supra-chondritic PGE patterns that are not simply predicted from modeled pristine mantle left after the core separation (Mann et al., 2012 *Geochim. Cosmochim. Acta.*). With devoting efforts to compile bulk-rock PGE data of worldwide mantle peridotites in the past decades, metasomatic PGE inputs have been postulated (e.g., Lorand and Luguet, 2016 *Rev. Mineral. Geochem.* and references therein). Recent approaches of *in-situ* analyses for base metal (Fe-Ni-Cu) sulfides (one of the representative PGE-host minerals) along with bulk-rock analyses supported such PGE mobility during metasomatic events (e.g., Alard et al. 2011 *J. Petrol.*, Delpech et al., 2012 *Lithos*). However, direct petrographic evidence for the metasomatic mobilization of PGE has not yet been documented because the samples are imposed on 'multiple' metasomatic events (e.g., Lorand et al., 2004 *Chem. Geol.*). Here we introduce sub-μm-scale investigations of 'armored' sulfide inclusion array of metasomatic origin within silicate mineral in a lherzolite xenolith. With employing analyses by a field-emission transmission electron microscope with energy dispersive X-ray spectroscopy (FE-TEM-EDS), we introduce direct evidence of PGE mobilization in response to a metasomatic event and delineate the mechanism of PGE migration in the mantle.

The lherzolite xenolith we use here was collected at Tahiti island. Since the lherzolite contains (1) vein-like clinopyroxenes in equilibrium with carbonaceous melt, (2) secondary CO_2 fluid inclusions, and (3) secondary carbonaceous silicate glass inclusions, we suppose that the lherzolite was subject to carbonatite metasomatism. Our intense investigations into sub-μm-sized sulfide inclusion array in a clinopyroxene crystal revealed that they partly coexist with carbonaceous aluminosilicate glass, implying that immiscible sulfide melt and carbonaceous aluminosilicate melt filled microcracks before hearing of the host clinopyroxene. From the fact that the sulfides contain appreciable amounts of Ir–Pt–Rh (~20 atomic%), we conclude that Ir, Pt and Rh were mobilized through carbonatite metasomatism. We speculate that the PGEs were transported via miscible carbonatite–silicate–sulfide melts, which reached a new immiscibility field owing to a decrease in pressure and temperature. Although immiscible sulfide melts were minor in volume, most of the PGE were partitioned into the sulfide melts.

Keywords: PGE, Metasomatism , Mantle xenolith, Sulfide, Carbonatite, TEM

Determination of the noble gas partition coefficients between metal-silicate melts using laser microprobe analysis

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Analyses of ocean island basalts (OIBs) reveal a geochemical reservoir characterized by unradiogenic, “primordial” noble gas signatures (e.g., high $^{3}He/^{4}He$ and low $^{40}Ar/^{36}Ar$ ratios), likely residing in the deep mantle. There has been much debate about the area holding the “primordial” noble gases deep in the Earth (Porcelli & Ballentine, 2002), including that the “primordial” noble gasses have been retained in the deepest region of the mantle since 4.4 Ga (Mukhopadhyay, 2012) or in the core since the core-mantle separation (Trieloff & Kunz, 2005). However, the validity of latter strongly depends on the quantity of noble gases the core incorporates during accretion and can hold in the present day.

In this study, in order to investigate noble gas partitioning behavior between the core and mantle, noble gases were dissolved into metal-silicate melts under high temperature and pressure conditions, and then the samples were quenched. Two series of sample synthesis were performed at different pressure-temperature ranges and experimental approaches. At the Geophysical Laboratory, Carnegie Institute of Washington, Ar partitioning experiments were conducted using a piston cylinder apparatus. Temperatures were 1700 ˚C, and pressures were 1 GPa. Experimental samples were contained by a double capsule: Pt outer capsule and graphite inner capsule. A Fe metal-silicate mixture was packed into the graphite capsule. Argon was added to the Pt outer capsule as a liquid, and the Pt capsule was welded shut while held in a bath of liquid N_2. At the Geodynamics Research Center, Ehime University, noble-gas doped hydrous silicate glass and iron were melted and equilibrated under high pressure and temperature (˜ 30 GPa, 1700 ˚C) using a laser-heated diamond anvil cell. After that, the noble gas concentrations contained in the each phase were analyzed using an ultraviolet laser ablation apparatus and a noble gas mass spectrometer at the University of Tokyo.

Preliminary results for argon showed that the partition coefficient D, where D = (noble gas in metal phase)/(noble gas in silicate phase), is in the order of 10^{-4}, which is three orders of magnitude lower than the previous work (Matsuda *et al.*, 1993). However, the apparent noble gas concentrations in the metal phase seem significantly controlled by contaminant phases, such as metal inclusions and micro- or nano-noble gas bubbles. Further experiments are necessary to distinguish noble gases dissolved in metal and retained in the contaminants to better constrain noble gas behaviors between silicate and metal.

References: Matsuda *et al.*, *Science* **259**, 788-791, 1993; Mukhopadhyay, *Nature* **486**, 101-104, 2012; Porcelli & Ballentine, *Rev. Mineral. Geochem.* **47**, 411-480, 2002; Trieloff & Kunz, *Phys. Earth Planet. Inter.* **148**, 13-38, 2005.

Keywords: core, mantle, noble gas, partition coefficient, high P-T experiment

Viscosity and atomic-local-structures of basaltic melt under high pressure

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High pressure properties of basaltic melt are of importance in deep Earth science related to such as early magma ocean and subsequent differentiation processes (Agee 1998; Ohtani and Maeda 2001; Suzuki, *et al.* 2005)
Recently, experimental studies reported that the viscosity of basaltic melt decreases with increasing pressure (Allwardt, *et al*. 2007; Sakamaki, *et al*. 2013). They suggested based on the results of classical molecular dynamics simulation (Nevins and Spera 1998) and ^{27}Al magic-angle spinning nuclear magnetic resonance (Allwardt, *et al*. 2007) that this anomalous behavior is related to the coordination change of Al. However, other silicate melts which contain none of Al also show a common behavior of viscosity (McMillan *et al*., 2009). It means that the microscopic origin of the anomalous pressure response of viscosity of the basaltic melt is still unclear. For this reason, in this study, we perform *ab initio* molecular dynamics simulations and analyze atomic–local-structures in basaltic aluminosilicate melt under pressure. At the last meeting, we reported the structural changes around Al atom. This time, we discuss relationship between the viscosity and structural changes not only around Al but other elements.

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Keywords: Ab initio molecular dynamics simulation, Basaltic melt, Viscosity , Microscopic structures

Viscosity of CO_2-bearing sodium aluminosilicate melt at high pressure

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Viscosity is one of the important transport properties controlling the migration of magma in the Earth's interior. Experimental and geochemical studies showed that magma in the deep interior was generated in the presence of CO_2. However, our knowledge on the effect of CO_2 on the viscosity of magma (silicate melt) is still insufficient. Here we report the viscosity of sodium aluminosilicate melt with jadeite composition containing 0.5 wt% of CO_2 under high pressure. Viscosity was measured by the falling sphere method by using X-ray radiography image. Experiments were carried out using the MAX-III apparatus installed at the station NE7A of PF-AR synchrotron radiation facility in KEK (High Energy Accelerator Research Organization), Tsukuba, Japan. Viscosity was calculated using the Stokes equation with the correction of wall effect. Viscosity measurements were carried out up to 2.4 GPa. We observed that viscosity of the CO_2-bearing melt was one order of magnitude lower than those of CO_2-free jadeite melt. The temperature dependence of the melt is similar to that of the CO_2-free jadeite melt.

Keywords: magma, volatile elements, carbon dioxide, maltle, high pressure, synchrotron radiation

Stability and thermos-elastic properties of iron oxide hydroxide: water transportation in the Earth's interior

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Hydrogen in the Earth’s interior plays an important role in the Earth’s interior, e.g., reduction of melting temperature and enhancing the deformation. Hydrogen is also a candidate of the light element in the core on the basis of melting experiments. Therefore, the stability and physical properties of hydrous minerals are fundamentally important. We found a high pressure polymorph of diaspore over 19 GPa and named δ-AlOOH (Suzuki et al., 2000). Crystal structure of δ-AlOOH was determined to be InOOH type with an orthorhombic unit cell. On the basis of the structural similarity between δ-AlOOH and a high pressure phase of SiO_2 with $CaCl_2$ structure, we estimated that δ-AlOOH is an important candidate of the water reservoir in the lower mantle.

A high pressure phase of iron oxide hydroxide, ε-FeOOH, has also an InOOH-related structure. Recently, high-pressure X-ray diffraction study of ε-FeOOH was carried out, and the pressure-volume-temperature (P-V-T) equation of state was determined (Suzuki, 2016). The P-V-T data up to 11 GPa and 700K fitted to a third-order Birch-Murnaghan equation of state yield: isothermal bulk modulus K_{T0} of 135(3) GPa; its pressure derivative K' of 6.1(9); $(\partial K_T/\partial T)_P$ of -0.05(2) GPa K^{-1}; a_0 of $2.6(7)\times10^{-5}$ K^{-1} and a_1 of $1.0(3)\times10^{-7}$ K^{-2}, where the volumetric thermal expansion coefficient is described as $\alpha_{0,T}=a_0+a_1\times(T\text{-}300)$.

Here we report the results of X-ray diffraction study on goethite. Experiments were performed by using a Kawai-type multi-anvil apparatus driven by a 700 ton uniaxial press on the station NE7A at PF-AR, a synchrotron radiation facility in KEK, Tsukuba, Japan. Powder X-ray diffraction data were collected by the energy-dispersive method using a Ge-SSD detector at a fixed diffracted angle 2 theta of 6.0 degree. Goethite (α-FeOOH) is stable at ambient condition. We observed transformation to ε-FeOOH at 7.8+-0.5 GPa and 873K. The reduction of volume by the transformation was about 3.5%. The P-V-T data of goethite were collected up to 7.55 GPa and 600 K. Fitting the volume data to the third-order Birch–Murnaghan EoS yielded an isothermal bulk modulus, K_0 of 85.9(15) GPa, and a pressure derivative of the bulk modulus, K', of 12.6(8). The temperature derivative of the bulk modulus, $(dK/dT)_P$, was −0.022(9) GPa K^{-1}. The thermal expansion coefficient a_0 was determined to be 4.0(5) $\times10^{-5}$ K^{-1}.

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. Goethite (α-FeOOH) transforms to ε-FeOOH at high pressure. At the core-mantle boundary, ε-FeOOH may react with the core, and oxygen and hydrogen are partitioned. We estimate that iron oxide hydroxide can transport hydrogen to the deep interior and supply hydrogen to the outer core. Also wüstite may be formed at the core-mantle boundary.

Keywords: mantle, hydrous phase, water, core, core-mantle boundary, high pressure

P-V-T equation of state of Al-bearing hydrous bridgmanite

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Water is the most abundant volatile component on the Earth. It has significant influences on the chemical and physical properties of mantle minerals (e.g., melting temperature, elastic properties, electrical conductivity, and so on.). The nominally anhydrous minerals(NAMs) can contain small amount of water. In particular, wadsleyite and ringwoodite which are the major constituent minerals in the Earth' s mantle transition zone can contain ~2-3 wt% water (e.g., Inoue et al., 1995; Kohlstedt et al., 1996). Recently, hydrous ringwoodite contained ~1.5 wt% water was discovered by Pearson et al. (2014) as inclusion in ultra-deep diamond. This observation implies that the mantle transition zone contains some water at least locally. On the other hand, water solubility of bridgmanite which is the most abundant mineral in the lower mantle, is a matter of debate (e.g., Bolfan-Casanova et al., 2000, 2003; Murakami et al., 2002; Litasov et al., 2003). In this situation, Al-bearing hydrous bridgmanite contained ~0.8 wt % water with 4.7 wt% Al_2O_3 was synthesized by Inoue et al., (in prep). However, the physical properties of Al-bearing hydrous bridgmanite under high pressure are unknown. Therefore, we clarified P-V-T equation of state of Al-bearing hydrous bridgmanite will be reported.

In situ P-V-T experiments of Al-bearing hydrous bridgmanite were conducted using multi-anvil high pressure apparatus (SPEED-Mk.II) with sintered diamond 2nd stage anvil at SPring-8 BL04B1. As we observed the dehydration of Al-bearing hydrous bridgmanite between 900 and 1500 K in our in situ open system experiment, we developed in situ closed system experimental method using Ag capsule. The experimental conditions were 35-45 GPa and 300-1500 K. In addition, the room temperature compression data of Al-bearing hydrous bridgmanite was obtained using diamond anvil cell (DAC) with He pressure medium at PF BL18C up to ~55 GPa in quasi-hydrostatic condition (Takemura, 2001).

The unit cell volume of Al-bearing hydrous bridgmanite decreased smoothly up to 52 GPa. This result indicated that the hydrogen bond symmetrization is not occurred at least up to 52 GPa at room temperature. The bulk modulus of Al-bearing hydrous bridgmanite is much smaller than that of Al-bearing anhydrous bridgmanite. In this presentation, we will report the thermo-elastic properties of Al-bearing bridgmanite in detail. Moreover, the water affect to physical properties will be discussed.

Keywords: bridgmanite, water, lower mantle, equation of state

Sound velocity of Al-bearing hydrous and anhydrous bridgmanites under high pressure

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Bridgmanite is a major constituent mineral in the lower mantle, and it is important to clarify the sound velocity to elucidate the mineral assembly (composition) of the lower mantle. Recently we reported that Al-bearing bridgmanite (Mg-silicate perovskite) can contain significant amount of water up to ~0.8 wt%, and confirmed the possible H position in the bridgmanite by means of the powder neutron diffraction analysis in J-PARC, together with the single crystal X-ray structural analysis in PF. Because of the H in the bridgmanite, the physical properties of the bridgmanite should be changed. So the determination of the effect of water for the sound velocity of bridgmanite is very important to discuss the possible water storage in the lower mantle.

For the comparison, the sound velocity measurement of anhydrous bridgmanite is also important. However, even in the anhydrous bridgmanite, the substitution forms are complicated. We recognize that both “Tschermak substitution” and “oxygen-vacancy substitution” forms exist in anhydrous bridgmanite. So the special attention was made to synthesize the two different anhydrous bridgmanites by preparing the appropriate compositional starting materials and conducting experiments in extremely anhydrous condition.

We succeeded to synthesize the polycrystalline hydrous and anhydrous bridgmanites using the Kawai-type high pressure apparatus (Orange 3000) in Ehime University suitable for the sound velocity measurements. In situ ultrasonic experiments combined with X-ray were conducted in BL04B1 beamline, SPring-8. In this talk, we will explain the experimental results in details.

Keywords: hydrous bridgmanite, anhydrous bridgmanite, lower mantle, Synchrotron X-ray in situ experiment, sound velocity

Development for hydrogen diffusion experiments under Ar/D_2 and D_2O condition

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There are many uncertainties about the origin of hydrogen in the earth. Especially, hydrogen isotopic compositions of the early earth are unclear. The characteristics of water of mantle in the early earth would be able to expect to estimate from those of hydrous minerals, for example, apatite crystals in the hadean and archean. However, without an understanding of hydrogen diffusivity in these hydrous minerals, it is difficult to esimate whether original hydrogen isotopic compositions from crystallization are preserved or the subsequently modified by reactions with water or H_2 gas after crystallization. Therefore, this study reports development of the diffusion experiment for hydrous minerals with diffusion source of water and Ar/D_2 gas.

The diffusion annealing system in this study could chose between D_2O line and Ar/D_2 line for the diffusion source. In addition, this system chose flow type and close type with vacuum system for the control of partial pressure in the crystal surface. Therefore, we need to estimate the residue of H2O and D_2O absorbed in the line and quarts tube when the Ar/D_2 gas line are selected.
The quantitative analyses for residue of absorbed water were estimated by annealing of apatite crystals in the different condition with the depth profile by Kyoto 4f-e7 secondary ion mass spectrometry (SIMS). This talk will discuss the results of different diffusion source in the apatite crystals and methods of control the partial pressure of Ar/D_2 diffusion experiments.

Keywords: Hydrogen, diffusion, SIMS

Lattice thermal conductivity of (Mg,Fe)O magnesiowustite

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The Earth has been cooling since it was born about 4.6 billion years ago. To decipher the thermal history of the Earth, thermophysical properties of the lower mantle materials that constitute more than half the volume of the Earth is of great importance. A number of research has suggested the possibility that (Mg,Fe)O ferropericlase, one of the main constituent minerals of the lower mantle, exists with very iron-rich chemical composition at the Earth’ s core-mantle boundary (CMB). Such iron-rich (Mg,Fe)O magnesiowustite at the CMB may cause regional variation of thermal conductivity of the lowermost mantle due to its distinct iron concentration, which potentially influences the mantle convection style, inner core age, inner core structure, geomagnetic field reversal frequency and so on [e.g. Olson, 2016]. However, there is no systematic study to examine the effect of iron on the thermal conductivity of (Mg,Fe)O solid solution under high pressure. In this study, we measured lattice thermal conductivity of (Mg,Fe)O magnesiowustite with various iron contents at high pressures, and evaluated its compositional dependence. Our results show much lower lattice conductivity of iron- rich magnesiowustite than that of MgO and FeO due to strong iron impurity phonon scattering, which would help to estimate the thermal conductivity of the expected iron- rich region in the lowermost mantle.

Reference: Olson, P. Mantle control of the geodynamo: Consequences of top-down regulation, *Geochem. Geophys. Geosys.* 17, 1935–1956, (2016).

Keywords: thermal conductivity, lower mantle, ferropericlase, magnesiowustite

Ab initio lattice thermal conductivity of MgO using a full solution to the linearized Boltzmann transport equation

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Lattice thermal conductivity, κ_{lat}, of MgO at high pressures and temperatures, up to 150 GPa and 4000 K, are determined using lattice dynamics calculations and the linearized phonon Boltzmann transport equation (BTE) beyond the relaxation time approximation (RTA) from first principles. It is found that the complete solution of the linearized BTE substantially corrects values of κ_{lat} calculated with the RTA by ~30%, from ~39 W m^{-1} K^{-1} to ~50 W m^{-1} K^{-1} under ambient conditions. The calculated values of κ_{lat} are in good agreement with those from the existing experiments. At conditions representative of the Earth’s core-mantle boundary (P = 136 GPa and T = 3800 K), κ_{lat} is predicted to be ~31 W m^{-1} K^{-1} and ~39 W m^{-1} K^{-1} by RTA and the full solution of BTE, respectively. We report a detailed comparison of our study with earlier theoretical studies.

Keywords: Lower mantle minerals, Lattice thermal conductivity, Computer simulation, Phonon-phonon interaction, Density-functional theory

Melting relations in the MgO-$MgSiO_3$ system under the lower mantle conditions

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Melting mechanism has important implication for chemical evolution of the Earth. Knowledge of the melting phase relation in the lower mantle is a key to understand the chemical differentiation in the early Earth and the nature of the ultralow-velocity zones (ULVZs) at the base of the mantle. While melting relations of mantle materials at relatively low pressure (below 30 GPa) have been extensively studied using a multi-anvil apparatus, the melting experiments at higher pressures are still limited. Only in a few model rock compositions, such as peridotite and mid-oceanic ridge basalt (MORB), the experiments were conducted under the CMB conditions using a laser-heated diamond anvil cell (LHDAC). Since chemical heterogeneity of both major elements and minor ones should have a large effect on the melting behavior, the melting phase diagrams as a function of composition are fundamental to understand the detail of the early melting history of the Earth and the nature of the ULVZs. In this study, we determined the melting relations in the MgO-$MgSiO_3$ system, which is a major component in the lower mantle.
The experiments were performed up to 115 GPa using a CO_2 laser heated diamond anvil cell. The quenched samples were polished and analyzed by a dualbeam focused ion beam (FIB) and a field emission scanning electron microscope (FE-SEM), respectively. The eutectic compositions and liquidus phase were determined on the basis of chemical and textual analyses of sample cross sections. Our experimental results show that the eutectic composition is Si/Mg molar ratio of ˜0.76 at around 35 GPa and it decreases with increasing pressure below 45 GPa. Above 45 GPa, it becomes relatively constant at about 0.64-0.65 Si/Mg molar ratio. Additionally, the eutectic composition was described by thermodynamic calculation under the whole lower mantle conditions. We obtained the Si/Mg molar ratio of ˜0.64 at the base of the mantle. The liquidus phase changes from MgO-periclase to $MgSiO_3$-bridgmanite at around 35 GPa in the Fe-free simplified pyrolite composition (˜0.7 Si/Mg molar ratio). In the other model rock composition such as chondrite (˜0.84 Si/Mg molar ratio), $MgSiO_3$-bridgmanite becomes the liquidus phase in the entire lower mantle. Thus $MgSiO_3$-bridgmanite should be the dominant phase to crystallize from a deep global magma ocean in the lower mantle.

Melting temperatures of MgO up to ˜50 GPa determined by micro-texture analysis

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Periclase (MgO) is the second most abundant mineral after bridgmanite in the Earth’ s lower mantle, and its melting temperature (T_m) under pressure is important to constrain rheological properties and melting behaviors of the lower mantle materials. Significant discrepancies exist between the T_ms of MgO determined by Laser-Heated Diamond Anvil Cell (LHDAC) and those based on dynamic compressions and theoretical predictions. We performed a series of LHDAC experiments for measurements of T_m of MgO under high pressure. The melting was detected by using micro-texture observations of the quenched samples.

We found that the laser-heated area of the sample quenched from the T_m in previous LHDAC experiments showed randomly aggregated granular crystals, which was not caused by melting, but by plastic deformation of the sample. This suggests that the T_ms of their study were substantially underestimated. On the other hand, the sample recovered from the temperature higher by 1500-1700 K than the T_ms in previous LHDAC experiments showed a characteristic internal texture comparable to the solidification texture typically shown in metal casting. We determined the Tms based on the observation of this texture up to ˜50 GPa.

Fitting our Tms to the Simon equation yields dT_m/dP of 103 K/GPa at zero pressure, which is consistent with those of the theoretical predictions (90˜120 K/GPa). Extrapolation of the present melting curve of MgO to the pressure of the CMB (135 GPa) gives a melting temperature of ˜7900 K. The high T_ms of MgO suggest the subducted cold slabs should have higher viscosities than previously thought, suggesting that the inter-connecting textural feature of MgO would not play important roles for the slab stagnation in the lower mantle. The present results also predict that the ultra-deep magmas produced in the lower mantle are perioditic, which are stabilized near the core-mantle boundary.

Keywords: Melting, Mineral physics, High pressure experiments

Phase relations of $MgSiO_3$-$FeSiO_3$ system up to about 60 GPa and 2300K using multianvil apparatus with sintered diamond anvils

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$MgSiO_3$ bridgmanite is the most abundant mineral in the Earth’s lower mantle, which can accommodate certain amount of $FeSiO_3$ under the P-T conditions of the lower mantle. Because of geophysical importance of $FeSiO_3$-bearing bridgmanite, phase relations of MgO-FeO-SiO_2 system have been investigated using both laser-heated diamond anvil cell (LHDAC) and Kawai-type multi-anvil apparatus (KMA), but there are some inconsistencies among their studies. Dorfman et al. (2013) made experiments up to 155 GPa and 3000 K using LHDAC, which reported a sharp increase of the solubility of the $FeSiO_3$ component in bridgmanite at 50-70 GPa. In contrast, Tateno et al. (2007) reported more continuous solubility of $FeSiO_3$ with pressure using similar techniques of LHDAC. On the other hand, Tange et al. (2009) precisely determined the phase relations in the system MgO-FeO-SiO_2 on the bases of KMA experiments using sintered diamond (SD) anvils, but the maximum pressure and temperature in this study were limited to 47 GPa at 1773 K.
Based on the newly developed high pressure and temperature techniques, we studied detailed phase relations in the system MgO-FeO-SiO_2 using KMA with SD anvils at pressures up to 61 GPa at a temperature of 2000 K. Synthetic pyroxene samples with chemical compositions of $(Mg_{0.4}Fe_{0.6})SiO_3$ and $FeSiO_3$ were used as the starting materials. Both quench experiments and in situ X-ray observations were adopted to constrain the phases present. Single-phase bridgmanite and an assemblage of wüstite + stishovite were formed in the $MgSiO_3$-rich and $FeSiO_3$-rich regions, respectively, under the present pressure and temperature conditions of up to ˜60 GPa, which is generally consistent with the phase relations in the earlier studies. We found the solubility of $FeSiO_3$ in bridgmanite increases almost linearly with increasing pressure from Fe* (Fe/Fe+Mg) = 0.19 for 27 GPa to 0.38 mole for 60 GPa at 2000 K. The iron content in wüstite also significantly increases from Fe* = 0.68 for 27 GPa to 0.96 for 60 GPa.

Keywords: bridgmanite, high temperature generation, sintered diamond anvil

Thai Seismic Array (TSAR) Project: Progress in FY2016

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The Thai Seismic Array (TSAR) project has started under the project "Seismic and geo-electromagnetic observation for core and mantle", which is one of the KAKENHI grants for an innovative area "Core-mantle co-evolution". In the JpGU2016 meeting, we reported the scope of the project, results of the site survey and status of the 2 pilot stations (Tanaka et al., 2016). In this presentation, we will show the progress in FY2016 and current status.

Since November 2016, we have started the deployment. As of February 13th, 2017, 30 stations are under operation, which are distributed in the central, northern, eastern, and northeastern Thailand. However, due to heavy rain and severe flooding in the southern Thailand in December 2016 and January 2017, we abandon the deployment of the stations in the Malay peninsula. Instead, we will construct a dense array in the central part of Thailand. The deployment of the additional 10 stations will be completed until the end of February.

Local strong slow S-wave anomalies at western edge of Pacific LLSVP

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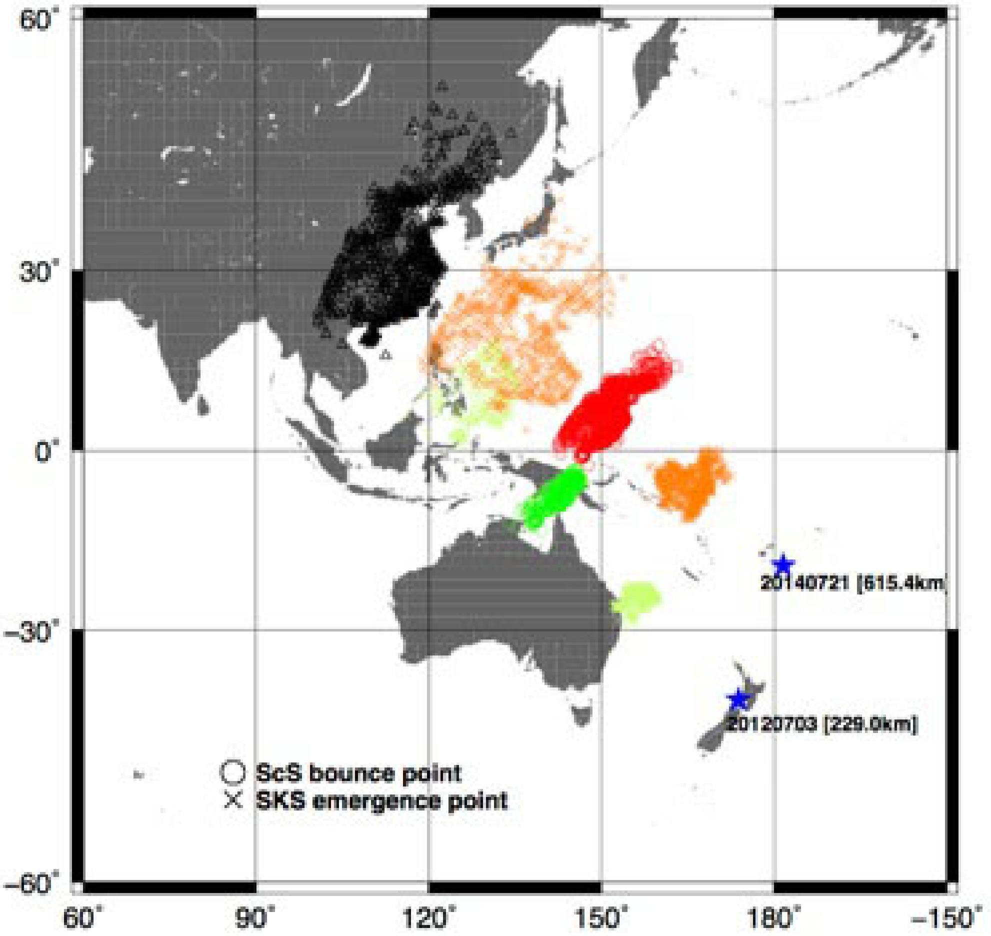
Seismic tomography studies have revealed two broad slow shear-wave speed anomalies regions beneath the Pacific and Africa called as LLSVPs (Large Low Seismic Velocity Provinces). There are geographic correlations between the LLSVPs and hotspots, and the LLSVPs could probably play an important role for convection throughout the mantle and thermal structure and evolution of the earth. The LLSVPs have been considered to be heterogeneous in composition since the boundaries between the normal mantle are sharp. To investigate the details of the sharp LLSVP edge we measure ScS–S and SKS–S differential traveltimes in the hypocentral distance of about 60 –90° using Japanese and Chinese seismic networks. We found anomalously large (more than 5 sec) ScS –S travel times accompanying normal SKS –S travel times, suggesting local strong slow region in the vicinity of the ScS bounce points (red circles in Figure 1). Such ScS bounce points locate to the northeast of New Guinea Island extending over 20 degrees in NE-SW direction. However below New Guinea Island, both ScS –S and SKS –S travel times are normal (green circles in Figure 1), indicating abrupt end of the local strong slow anomalies.

Keywords: core mantle boundary, LLSVP, ScS wave, SKS wave



Waveform tomography for 3-D shear velocity structure in the lowermost mantle beneath the Northern Pacific

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We conduct waveform inversion (Kawai et al. 2014, GJI) to infer the 3-D SH-velocity structure in the lowermost mantle beneath the Northern Pacific, using ~20,000 transverse components of broadband body-wave seismograms for the first step. We use S, ScS and other phases that arrive between them. The 3-D SH-velocity models obtained by our inversion show three prominent features: (i) horizontal high-velocity anomalies up to about 3 per cent faster than the Preliminary Reference Earth Model (PREM) with a thickness of a few hundred km and a lower boundary which is at most about 150 km above the core-mantle boundary (CMB), (ii) low-velocity anomalies about 2.5 per cent slower than PREM beneath the high-velocity anomalies at the base of the lower mantle, (iii) a thin (about 200 km) low-velocity structure continuous from the base of the low-velocity zone to at least 400 km above the CMB. We interpret these features respectively as: (i) remnants of slab material where the Mg-perovskite to Mg-post-perovskite phase transition could have occurred within the slab, (ii,iii) large amounts of hot and less dense materials beneath the cold paleoslab remnants just above the CMB which ascend and form a passive plume upwelling at the edge of the slab remnants (Suzuki et al. 2016, EPS).

As a second step, we conduct waveform inversion using both the transverse and radial components to infer the more detailed isotropic shear velocity structure in the lowermost mantle beneath the Northern Pacific. We also infer the transversely isotropic (TI) shear-velocity structure for this region using two horizontal components. We conduct synthetic resolution check to examine the ability of our methods and dataset to resolve the TI shear-velocity structure.

Keywords: Lowermost mantle, Waveform inversion, Shear velocity structure

3-D S-velocity velocity structure in D″obtained by waveform inversion after redetermination of the earthquake source parameters

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Our group previously investigated the 3-D S-velocity structure within the D″ layer beneath central America using waveform inversion (Kawai et al. 2014, GJI; Borgeaud et al. 2016, JPGU). In these studies, the source parameters were fixed to the Global Centroid-Moment-Tensor (GCMT) Project solutions. The GCMT solutions are determined using not only body-waves, but also surface-waves, and mantle-waves, and the data are filtered in a different frequency range from that used in our waveform inversion studies. In this study we redetermine the CMT solutions using body-wave data only, filtered in the same frequency range (12.5-200 s) as that used in our waveform inversion studies. Then, we re-infer the 3-D S-velocity structure of the D″ layer beneath central America using the new CMT solutions. We compare the respective 3-D models to see whether (1) waveform inversion is robust to small changes in the source parameters, and (2) whether the models obtained by waveform inversion are improved by using the redetermined source parameters. We find that the variance reduction for the model inferred using our redetermined CMT solutions is better than that for the model inferred using the GCMT solutions. Also, although this is somewhat subjective, the new 3-D model appears to provide sharper images with a better visualization of paleoslab-like high-velocity structures.

Keywords: Waveform inversion, Earthquake source parameters, Seismic velocity structure of D″

D111-type guide block for high-pressure deformation experiments

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For accurate understanding of material and heat transports in the Earth's interiors, knowledge of rheological property under high-pressure and high-temperature is indispensable. To study rheological property of materials at high-pressure quantitatively, deformation experiments has been carried out using various deformation devises including rotational Drickamer apparatus and deformation-DIA apparatus. Recently a new type apparatus, deformation T-Cup (DT-Cup), which is based on Kawai-type multi-anvil apparatus was developed by Hunt et al. (2014). In the DT-Cup, by driving two second-stage anvils using differential actuators, well-controlled deformation experiments can be conducted up to confining pressure of 18 GPa. However, more improvement is needed to achieve deformation at the condition of the Earth's lower mantle (>23 GPa).
To study the rheological property at the lower mantle condition experimentally, we are planning to install a “D111-type guide block” on a synchrotron beamline NE7A at PF-AR, KEK, Tsukuba. By combining D111-type guide block with the MAX-III press, it acts as a deformation apparatus (D111-type deformation device) that is improved version of DT-Cup. The our D111-type device can be used under higher press load (max. 700 tonf) which enables us to conduct quantitative deformation experiments at the lower mantle pressures. Stress and strain during deformation can be measured in situ using the monochromatized synchrotron X-ray. The installation of the D111-type guide block is planned on March 2017. We expect fruitful results on the deep Earth rheology based on experiments using the D111-type device in near future.

Keywords: deformation experiments, deep Earth rheology , lower mantle

Toward the in-situ deformation experiments under the lower mantle conditions using D-DIA apparatus

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Rheological properties of lower-mantle forming minerals such as bridgmanite are important to understand the cause of seismic anisotropy and the viscosity structure in the lower mantle. To explore the creep behavior and crystallographic preferred orientation of high-pressure minerals, two types of deformation apparatus, namely, the D-DIA type (Wang et al., 2003) and the rotational Drickamer apparatus (RDA: Yamazaki and Karato, 2001) have been adopted to deformation experiments at high pressures. Even though the upper limit of confining pressure is 4 GPa in the Griggs rig (e.g., Rybacki et al., 1998), the upper limit is more than 18 GPa in the case of D-DIA and RDA (Miyagi et al., 2013; Kawazoe et al., 2016). Recently, Girard et al. (2015) and Tsujino et al. (2016) succeeded to deform bridgmanite at lower mantle pressures and temperatures using a RDA and a Kawai-type apparatus for triaxial deformation (KATD: Nishihara, 2008), respectively. Even though the pressure and temperature conditions available in a RDA and a KATD have been extended to the lower mantle conditions, in-situ D-DIA experiments are still limited to the conditions of lower part of the mantle transition zone (Kawazoe et al., 2016). The main cause disturbing further pressure generation using an in-situ D-DIA apparatus is relatively low toughness of the x-ray transparent anvils made from sintered diamond or cubic BN. In the geometry of cubic-type multianvil apparatus, the available press load needs to be low (< 0.6 MN) to avoid the breakage of the x-ray transparent anvils. Also, conventional WC anvils are not suitable for the generation of lower mantle pressures in the geometry of cubic-type multianvil apparatus. The advantages of D-DIA apparatus are as follows: i) sample deformation can be precisely controlled by two deformation rams (i.e., deformation with a constant strain rate) and ii) temperature can be monitored by using a thermocouple. To explore the quantitative deformation experiments at lower mantle conditions, we adopted the 'jacketed' 6-6 type anvils (Yamada et al., 2016) and optimized the cell assembly using preformed gaskets (e.g., Kawazoe et al., 2010). Combining these techniques, we succeeded to generate 24 GPa at room temperatures using a D-DIA apparatus. Pressures higher than 20 GPa are also available with our in-situ experimental setup, suggesting a possibility of quantitative deformation experiments at lower mantle conditions in near future.

Keywords: D-DIA apparatus, lower mantle, 6-6 type anvil

Sulfur distribution between basaltic magma and Fe-FeS melt

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Earth is consist of crust, mantle, and core. The crust and mantle are made of silicates and oxides. The core is mainly composed of iron with light elements such as H, C, O, S, and Si. This is because the density of the core is smaller than that of pure iron under the core conditions. The Earth’s structure was considered to have formed during the differentiation of magma ocean in the early stages of formation of Earth. During the magma ocean, the metallic liquid reacted with the magma at the bottom of the magma ocean.

Since sulfur is depleted in the mantle compared to CI chondrites (e.g., Murthy and Hall, 1970) and sulfides are found in meteorites, sulfur is one of the most plausible candidate elements in the Earth’s core. Therefore, the study on Fe-S system provides us some significant information about magma ocean and core formation. In magma ocean, metallic melts sank to the bottom of the magma ocean because of gravitational separation. At the same time, a partitioning between liquid silicate and liquid metal occurred under very high temperature and pressure conditions. Sulfur distribution and isotope fractionation are affected by these parameter (T, P, f_{O2} etc.). Therefore, research on sulfur distribution leads to understanding the process of the differentiation between core and mantle in early Earth.

In this study, partitioning experiments between silicate (basaltic composition) and metal (Fe-14 wt%S alloy) were performed using Kawai-type 3000 ton multi-anvil press at Tohoku University. The experiments were carried out at pressures ranging from 1 to 7 GPa and heated to temperatures of 1400 °C to 1800 °C. Chemical composition of the sample were analyzed using SEM-EDS.

Experimental results show that correlations between distribution coefficients of sulfur and temperature changed by pressure. Distribution coefficients of sulfur at 3 GPa decreased with increasing temperature while those at 5 GPa increased with increasing temperature. Also, correlations between distribution coefficient of sulfur and pressure were changed by temperature. Distribution coefficients of sulfur at 1650 °C increased with increasing pressure, on the other hand, those at 1800 °C decreased with increasing pressure. As a whole, it was observed that they had a negative relation between distribution coefficient and temperature, and a positive relation between distribution coefficient and pressure.

The average distribution coefficients in this study was 76±36. McDonough (2003) reported that the total abundance of sulfur in Earth was 6530 ppm. Using the average and the abundance, we estimated that the amount of sulfur in Earth’s mantle was 82±7 ppm. This abundance is less than expected previously (e.g., Palme and O’Neill, 2001; McDonough, 2003). However, it is actually expected to be higher content of sulfur in Earth’s mantle because magma ocean experienced higher temperature condition than this study, with higher lithophile nature. Oxygen fugacity is also an important parameter that influence element partitioning. Under reducing condition, sulfur tends to be distribute to silicate phase than in oxidizing condition. The present ΔIW (oxygen fugacity to Iron-Wüstite buffer) of the experiments were in the range of -1.16 and -1.44. Assuming more reductive condition than the present ΔIW in magma ocean, the content of sulfur in Earth’s mantle might increase and match the geological estimate.

Outer core composition estimated from thermoelastic properties of liquid Fe alloys

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The Earth's core is thought to include substantially large amounts of light elements (LEs), which account for observed density deficits of ~10% for the liquid outer core and ~5% for the solid inner core (e.g. Birch, 1964; Brown and McQueen, 1986; Jephcoat and Olson, 1987; Uchida et al., 2001; Anderson et al., 2003; Dewaele et al., 2006; Ichikawa et al., 2014). The density jump across the inner-outer core boundary (ICB) evaluated by seismic wave observations is ~4.5-6.7 % (Shearer and Masters, 1990, Masters and Gubbins, 2003), which cannot be accounted for by the melting phase transition of pure iron alone and requires a LEs partitioning more into the outer core (Alfè et al., 2002a). Although oxygen, silicon, carbon, nitrogen, sulfur, and hydrogen have been proposed as candidates for the LEs (Stevenson, 1981), little is known about the amount and the species so far. However, experimental determination of these properties for the liquid states are still not practical at the outer core pressure and temperature (from ~136 GPa to ~329 GPa and from ~4,000 K to ~6,000 K) due to technical limitations. The ab initio density functional computation method is instead quite powerful to investigate liquid properties under such extreme condition. Here, we show integrative analyses of the compositional model of the Earth’s outer core based on the ab initio thermoelasticity of iron-nickel-LE alloy liquids. Results indicate that combination of LEs in the outer core cannot be fully constrained only by the comparison between elastic properties and seismic observation. Comprehensive considerations covering density jump at the ICB, phase relations, geochemical constraints, and the ΔV_P of low-velocab initioity anomalies in the outermost core are used to refine the compositions of the outer core.

Keywords: Composition of the Earth's outer core, Light elements, ab initio molecular dynamics simulation

Density of Fe-FeS binary melts at high pressures

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Magnetism of small planetary bodies such as Mercury and Ganymede is thought to be originated from core dynamo driven by chemical convection, which is connected with Fe-snowing in the liquid core. Fe snowing phenomenon is governed by both the adiabat in the liquid core and the melting slope of the constituent substance of the core. Thus, it is fundamental to study the density and thermal expansivity of liquid iron alloy under pressure to understand Fe-snowing phenomenon. Sulfur is thought to be a primary lightening element in the metallic core of the small planets, satellites and planetesimals. Here we report the results of density measurements of Fe-FeS binary melts at high pressure by means of X-ray absorption technique. Experiments were conducted at BL22XU of SPring-8, at which the cubic-type multi-anvil press is equipped and the highly brilliant monochromatic X-ray is available. We determined the densities and the thermal expansivities of Fe-S liquids at about 3.5 GPa and 1500-2000 K. Density of Fe-S liquid increases with Fe content and the mixing of Fe and FeS liquids does not deviate much from the ideal solution. Our new data would contribute to understand compression behavior as well as thermochemical properties of Fe-S liquids alloys under pressure.

Keywords: planetary core, Fe-S liquids, density, thermal expansivity

Sound velocity and density of liquid iron alloys under Earth’ s core pressures by laser-shock compression

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Sound velocity at Earth’ s core conditions are one of the most important physical properties in Earth science because it can be directly compared with the seismological Earth model (PREM: Preliminary Reference Earth Model) [1]. The composition of solid inner core is estimated from the comparison of the model [1] and the extrapolation of sound velocities as a function of density of iron and iron alloys obtained by the static compression experiment [2, 3]. Birch’ s law, a linear sound velocity–density relation [4], is used to extrapolate sound velocities to densities in the core condition. On the other hand, the composition of liquid outer core is estimated from the partitioning and solubility data in the inner core boundary condition for the composition of solid core. There has been some works for the sound velocity of iron and iron alloys on the Earth’ s core condition by dynamic techniques using explosive [5], gas gun [5-9], and laser [10-12]. Huang et al. estimated that the outer core composition is Fe with 0.5 wt.% O and 9.5 wt.% S by the comparison of PREM and sound velocities of Fe-S-O system [9]. In this study, we measure the sound velocity and density of liquid iron alloys by shock-compression method using high-power laser.

We conducted shock-compression experiments using a High Intensity Plasma Experimental Research (HIPER) system at the GEKKO-XII laser irradiation facility [13] at the Institute of Laser Engineering, Osaka University. The samples were Fe-Ni alloys, Fe-Si alloys, and pyrrhotite. The sound velocities and densities of shock-compressed iron alloys using the high-power laser were measured by x-ray radiography [10-12] at pressures up to 1000 GPa.

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Keywords: Sound velocity, Shock compression, Iron alloy, Earth's core, Birch's law

Anomalous behavior of core phase PKP*bc-df* differential travel times from observations of South Sandwich Islands earthquakes by Alaskan and US seismic arrays

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We report anomalous behavior of core phase PKP*bc-df* differential travel times recorded by stations of the Alaska regional network and current USArray for several South Sandwich Islands (SSI) earthquakes. The data sample the inner- and outer-core for the polar paths, as well as the lowermost mantle beneath eastern Alaska. Our major observations are: (1) the fractional travel time residuals of PKP*bc-df* (residual divided by PKP*df* travel time in the inner-core) increase rapidly from 147°to 149°(up to 0.01, corresponding to travel time of ~1s), and keep almost constant after 149°. (2) From southwest to northeast, there is a decrease in fractional residual at distance larger than 150°. Either a rapid velocity change in the uppermost inner core or existence of a large lateral velocity variation at lowermost mantle, which is seen in a recently tomography model (Young et al., 2013), may explain the observation. The preliminary analysis indicates that modeling for discontinuities with different velocity jump in the inner-core does not seem to reproduce the observed fractional residuals, and that it may suggest a probable complexity at lowermost mantle. One possible interpretation is that PKP*bc* and PKP*df* sample different portions of the heterogeneity at larger distance, which results in the sudden increase of the fractional residuals. The large residuals observed from the polar path data for SSI events are usually explained by strong anisotropy in the uppermost inner-core, which might have been misinterpreted if its affected by some structure at the lowest mantle. Further work including waveform modeling is need to resolve what causes the anomalous behavior of our observation.

Sound velocity of hcp-Fe at multi-megabar pressures

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Earth’ s inner core consists of mainly hexagonal close-packed iron (hcp-Fe). Therefore, the physical properties of hcp-Fe can provide significant knowledge about the core. Despite seismological observations providing density-sound velocity data of Earth’ s core, there are few experimental reports about the sound velocity of hcp-Fe at ultrahigh pressure. Direct comparison of the sound velocity of hcp-Fe with that of observed inner core can provide a clear difference between them, which is an important information to determine the core composition. Here, we report the compressional sound velocity (V_P) of hcp-Fe up to 250 GPa using an inelastic X-ray scattering technique at BL43LXU of SPring-8. Based on the data, we can provide a standard of hcp-Fe (a linear relation of V_P with density: Birch’ s law), which enables us to indicate a better constraint on the composition of the Earth's core.

Keywords: core, sound velocity, high pressure

Sound velocity of iron-nickel alloys determined by femtosecond acoustic measurement in diamond anvil cell

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Iron-nickel (Fe-Ni) alloy is believed to be a major component of the Earth's core based on the cosmochemical models and the studies of iron meteorites, although accurate chemical composition of the Earth’s core is still unknown. Comparison between seismic wave velocity profile in the Earth and laboratory data of sound velocity of Fe alloys enables us to decipher chemical composition and comprising minerals there. Acoustic velocity of $Fe_{0.92}Ni_{0.08}$ has been obtained from nuclear resonant inelastic x-ray scattering (Lin et al., 2003), while experimental study on sound velocity of Fe-Ni alloy has not been performed in a wide range of nickel content. Here we measured longitudinal wave velocities of Fe, $Fe_{0.95}Ni_{0.05}$ and $Fe_{0.85}Ni_{0.15}$ up to 61 GPa and 300 K by means of a femtosecond acoustic technique in a diamond anvil cell (Decremps et al., 2014). The obtained sound velocity of Fe is in good agreement with previous studies. We also found that the acoustic velocities of iron-nickel alloys are slightly lower than that of pure iron.

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Keywords: core, sound velocity, iron-nickel alloy, high pressure

Atomic diffusion in solid iron at Earth’ s inner core conditions

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Crystalline iron is the main constituent of the Earth’ s inner core[1]. The thermomechanical properties of solid iron at high pressure and temperature therefore mainly control the dynamics and evolution of the inner core. One of those properties is atomic diffusion which plays a key role in many processes, such as plastic deformation (viscosity) and crystal growth. Ongoing debate about the seismologically observed elastic anisotropy of the Earth’ s inner core[2,3] has led to several suggestions whether to find its origin in non-uniform core growth[4], dendritic crystal growth[4,5] (core solidification) or in solid-state flow[4,6,7] (formation of LPO), all which depend on atomic diffusion processes. In addition, the diffusion anisotropy of iron at inner core conditions provides a link between seismic anisotropy and plastic deformation of the inner core. Therefore, a thorough understanding of atomic diffusion mechanisms in iron polymorphs is essential to gain better insight into the evolution of the Earth’ s inner core.
Since experiments are extremely difficult to perform at inner core pressure and temperature conditions, computational mineral physics provides an alternative to study atomic diffusion in iron under those conditions. In this work, the effect of pressure on vacancy diffusion is investigated by means of defect energetics as it largely determines the rate of vacancy diffusion. First principles simulations have been performed to calculate activation enthalpies for self-diffusion in FCC- and BCC- and HCP-Fe at a pressure range up to the conditions of the Earth’ s inner core. Our results show that pressure significantly increases defect energetics and in particular is responsible for suppressing defect concentration substantially in iron at inner core conditions. Consequently the rate of vacancy diffusion will be strongly inhibited. Intrinsic vacancy concentration plays an important role in metals in contrast to ionocovalent minerals where extrinsic vacancy concentration may determine effective vacancy diffusion. The question then arises whether other mechanisms allow to enhance vacancy concentration in iron under inner core conditions. If not, the latter will have direct consequences for the interpretation of the seismologically observed inner core anisotropy in terms of intracrystalline plasticity.

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Keywords: Earth's inner core, atomic diffusion, plastic deformation

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

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The Earth's core has supposed to be constituted by iron, nickel and some light elements. In order to elucidate the property of the Earth's core, many studies to quantify the content of light elements in the Earth's core has been progressed through sound velocity and magnetic measurements, or theoretical research. Hydrogen is one of the most probable candidate among the light elements constituting the Earth's core due to the relations between iron and hydrous melt in the magma ocean in the early Earth, and the discovery of the post-perovskite phase and that melting temperature. Although several studies on iron hydride (FeH_x) have been conducted, precise measurement of hydrogen content in metallic iron under high pressure and high temperature conditions has not been conducted due to the difficulty of the experiment. Hydrogen cannot be directly observed by traditional methods such as x-ray diffraction method. On the other hand, in neutron diffraction experiments, most of the direct observations of hydride has been carried out through substitution from hydrogen to deuterium because hydrogen has strong incoherent scattering. Therefore in many previous studies, the volume and the content of the hydrogen in metallic iron are assumed through the studies of several metallic hydride. However, such assumptions without precise measurement cause uncertainty, for example, when deriving the hydrogen content from the volume of FeH_x. In this study, to determine the hydrogen content and volume at high pressure and high temperature, high pressure neutron diffraction experiment for FeH_x was conducted under nearly isobar condition at 5-6 GPa and 8-9 GPa up to 1100 K in BL11 beamline, J-PARC. The phase transition and hydrogenation of iron were observed by dhcp-FeH_x and fcc-FeH_x phases, which are high pressure and high temperature phase of FeH_x. The structure of FeH_x and the content of hydrogen were determined by Rietveld refinement. The content of hydrogen *x* was obtained to 1.0-0.5, which is decreased by increasing temperature. We report the relations between the volume and the content in FeH_x at high pressure and high temperature.

Keywords: Iron hydride, Neutron diffraction, High pressure

The band structure and impurity resistivity of hcp and fcc Fe based alloys: Implications for planetary cores

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It is widely known that the Earth’ s Fe dominant core contains a certain amount of light elements such as H, C, N, O, Si and S (e.g. Hirose et al., 2013). The electronic band structure of Fe provides fundamental thermodynamic quantities (e.g. Boness et al. 1986). Gomi et al. (2016) calculated the band structure of substitutionally disordered hcp Fe-Si and Fe-Ni alloys, which suggest the broadening of the band structure due to Si is related to the impurity resistivity. However, only a few studies have investetaged the effect of alloying. In this study, we report the results of first-principles calculations on the band structure and the impurity resistivity of substitutionally disordered hcp and fcc Fe based alloys.

The first-principles calculation was conducted by using the AkaiKKR (machikaneyama) package, which employed the Korringa-Kohn-Rostoker (KKR) method with the atomic sphere approximation (ASA). The local density approximation (LDA) was adopted for the exchange-correlation potential (Moruzzi et al., 1978). The coherent potential approximation (CPA) was used to treat substitutional disorder effect (e.g. Akai, 1989). We mainly focused on Si, Ni, C, N, O and S impurity elements. The impurity resistivity is calculated from the Kubo-Greenwood formula with the vertex correction (Butler, 1985; Oshita et al., 2009; Gomi et al., 2016).

In dilute alloys with 1 at.% impurity concentration, calculated impurity resistivities of C, N, O, S are comparable to that of Si. On the other hand, in concentrated alloys up to 30 at%, Si impurity resistivity is the highest followed by C impurity resistivity. Ni impurity resistivity is the smallest. N, O and S impurity resistivities lie between Si and Ni. Impurity resistivities of hcp-based alloys show systematically higher values than fcc alloys. We also calculated the electronic specific heat from the density of states (DOS). For hcp and fcc Fe, the results show the deviation from the Sommerfeld value at high temperature, which is consistent with previous calculation (Boness et al., 1989). However, the degree of deviation becomes smaller with increasing impurity concentration.

The violation of the Sommerfeld expansion is possible source of the violation of the Wiedemann-Franz law (Gomi and Hirose, 2015; Secco et al., 2017), but the present results predict that the effect may not significant. Therefore, we conclude that the combination of the Wiedemann-Franz law and the resistivity saturation (Gomi et al., 2013; Ohta et al., 2016) can reasonably predict the thermal conductivity of the Earth’ s and planetary cores.

Keywords: core, electrical resistivity, band structure, KKR-CPA

Phase relations in the Fe-FeSi system at 10 GPa : Implications for Mercury’s core

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Mercury’s magnetic field, which shows dipole, has been observed by Mariner 10. Core dynamo is the most reliable model for generating the dipolar magnetic field. A high electrical conductive fluid, i.e., a liquid core, plays an important role for generating the core dynamo. Assuming the pure iron core, the present core would be completely solidified based on the Mercury’s thermal history. Therefore, other factors are needed to maintain the molten Mercury’s core. One of the most plausible factor is a depression of the melting point of pure Fe core due to dissolving light elements. Recent studies have suggested that Mercury’s core may contain several wt% silicon based on high-pressure experiments. Therefore, the melting relations of the Fe-FeSi system at high pressures can provide knowledge of the Mercury’s core structure. However, high-pressure phase relations of this system are not yet known precisely. In order to get the better understanding of the core structure, it is needed to perform melting experiments under the core conditions.

In this study, we determined the phase diagram for the Fe-FeSi system at a pressure of 10 GPa and temperatures between 920 ℃ and 1800 ℃ based on in-situ X-ray and quenched experiments using a Kawai-type multi-anvil apparatus. Our results showed that the system had two eutectic points at approximately 10 wt% Si and 20 wt% Si and sub-solidus phases are fcc-Fe (<10 wt% Si) and Fe_3Si (10-20 wt% Si) and FeSi (>20 wt% Si). Based on our results, we suggest three models of Mercury’s core evolution depending on the initial core composition.

Keywords: Mercury’s core, Iron-silicon alloys, Phase diagram, High pressure

Experimental investigation into the cause of a high attenuation zone of the lunar seismic waves: A possible partialy molten layer at the lowest lunar mantle

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Existence of a partially molten layer at the lunar core mantle boundary is suggested by recent seismic studies. It is important to study experimentally the chemical and physical condition at the boundary. However, the chemical compositions of the lunar mantle are still poorly understood. There is a long-standing hypothesis that dense Ti-rich cumulate minerals were crystallized from the lunar magma ocean at shallow depth (~100 km) at the final stage of the lunar formation history. Furthermore, those minerals subsequently sank deep into the moon because of gravitational instability. Convective mixing of the late and early cumulates could result in a hybrid lunar mantle.
In this study, high temperature (1200 - 1500°C) and high pressure (4 - 5 GPa) experiments are conducted to investigate the solidus of the lunar lowermost mantle which could be composed of the mixture of the late and early cumulates. The composition of the late cumulate suggested by Elkins-Tanton et al. (2011) was selected in this study. The solidus temperatures were determined to 1225 ±10°C at 4 GPa and to 1275 ±25°C at 5 GPa, defining a slope for the solidus of 5 °C/ kbar. Based on the solidus temperatures determined in this study, melting temperature at lunar core- mantle boundary (approximately 4 - 5 GPa) can be extrapolated as 1225-1275 °C, which is also lower than previous studies (e.g. Van Orman and Grove, 2000; Thacker et al., 2009).
Because the lower limit temperature at lunar core-mantle boundary (e.g. Flourish and Nakamura, 2009), which was estimated by terrestrial heat flow and seismic studies, has been reported to be higher than the solidus of the later cumulates determined in this study. Therefore, later cumulate could be a strong candidate for component of partial molten layer at lunar core- mantle boundary.

Keywords: core-mantle boundary, low-velocity zone, partial melt

Melting experiments of plagioclase under the shock-vein conditions

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High-pressure phase transitions of minerals have been frequently observed in heavily shocked meteorites, mainly within or around the shock veins (e.g., Chen et al. 1996). The plagioclase entrained in or adjacent to the shock veins transformed into maskelynite (e.g., Chen and El Goresy 2000), lingunite (e.g., Gillet et al. 2000) or jadeite plus amorphous materials (Miyahara et al. 2013). These transformations likely occurred in solid state, and the processes could be highly affected by the crystallization kinetics, as demonstrated by the kinetics studies of Kubo et al. (2010, 2016) at 18-25 GPa below 1673 K. On the other hand, the shock-metamorphic products of plagioclase exhibit some melting features (e.g., Chen and El Goresy 2000), and it is also likely that the shock metamorphism of plagioclase proceeded under the shock-vein conditions, typically 20-24 GPa and 2273-2673 K (Chen et al. 1996). Thus, high-temperature studies are necessary for further understanding the shock metamorphism of plagioclase in heavily shocked meteorites.

In this study, subsolidus and melting phase relations of $Ab_{85}An_{10}Or_5$ (oligoclase, the typical composition for the plagioclase found in heavily shocked meteorites) have been investigated by multi-anvil experiments at 16-23 GPa and 2273-2700 K. At 19-22 GPa, the subsolidus phase assemblage of $Ab_{85}An_{10}Or_5$ is jadeite (Jd) + stishovite (St) + hollandite (Holl) + CAS phase, and the melting sequence is Jd (the solidus phase), Holl, CAS phase and St (the liquidus phase). The liquidus temperature of $Ab_{85}An_{10}Or_5$ is at least 100 K higher than that of KLB-1 peridotite at 19-22 GPa. If the liquidus temperature of KLB-1 peridotite is used to infer the shock-vein temperatures, and if oligoclase completely melted at 19-22 GPa during impact, the oligoclase needed to be hotter than the shock veins, and therefore a localized heating in oligoclase is essential. It is found that Na-rich Holl and Na-rich CAS phase are stable in the composition of $Ab_{85}An_{10}Or_5$ at 22 GPa and ˜ 2500 K; the silicate liquid formed by melting crystallized into Holl, CAS phase and St during quenching. These phenomena likely relate with the natural occurrence of lingunite (e.g., Gillet et al. 2000) and CAS phase (Beck et al. 2004) in heavily shocked meteorites, but the kinetics problem must be further discussed. In addition, the intergrowth of CAS phase and St observed in some Martian meteorites (Beck et al. 2004) has been reproduced by quenching a labradorite melt at 23.5 GPa.

Keywords: Plagioclase, High Pressure and High Temperature, Phase Relation, Shock Metamorphism