High-P,T elasticity of hcp iron

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Earth’s inner core (329~364 GPa and 5000~6000 K) is known to be composed of hexagonal closed pack (hcp) structured solid Fe-Ni alloy and seismologically anisotropic. Thermoelasticity of hcp (c) iron is therefore a key to interpreting seismological information of the inner core. Since experimental measurements are still technically impractical, theoretical approaches in particular ab initio density functional computation have substantial roles. There are two different ways to simulate high-P,T elastic constants (cᵢⱼ) of crystals. One is based on the lattice dynamics method + quasiharmonic approximation (Sha and Cohen, 2010a,b) and the other is based on the molecular dynamics method (Vocadlo et al., 2009; Martorell et al., 2013). The former and the latter basically fail to capture higher-order anharmonicity and low-temperature quantum effects, which would be substantial and marginal in subsolidus condition, respectively. Due to these problems, distinct differences can be seen in high-P,T cᵢⱼ and their temperature dependences calculated by these different approaches. In this study, we performed ab initio molecular dynamics simulations employing a supercell containing 96 Fe, which is 50% larger than in the previous study with 64 atoms (Vocadlo et al., 2009; Martorell et al., 2013), to check the previous results. Technical details for computing high-P,T cᵢⱼ are basically the same as in our previous studies (Ichikawa et al., 2014; Kawai and Tsuchiya, 2015). We will present temperature dependences of elastic wave velocities and their anisotropies at the Earth’s inner core pressures over 300 GPa.


Keywords: Ab initio calculation method, Hcp iron, Elasticity, Earth’s inner core
Hydrogen is one of the most important candidates of light element(s) of the components the core of the Earth which explain the density deficit of the core. During the core formation, hydrogen preferentially dissolved into the metallic core as FeH$_x$ (e.g. Fukai, 1984; Okuchi et al., 1997). However, the phase diagram of FeH$_x$ is limited to relatively low pressure (Sakamaki et al., 2009), and its crystal structure under core pressure and temperature has not been revealed. Energetic calculations indicate the transition of double-hexagonal close packed (dhcp) to hexagonal close packed (hcp), and hcp to face-centered cubic (fcc) structure at lower mantle pressure (Isaev et al., 2007), but it has not been verified by experiments. We examined the phase transition from dhcp- or hcp-FeH$_x$ to fcc-FeH$_x$ by high-pressure and temperature experiments using laser-heated diamond-anvil cell technique and synchrotron X-ray diffraction measurements at SPring-8. It was revealed that dhcp-FeH$_x$ disappeared and hcp-FeH$_x$ formed at \~60$\text{ GPa}$, and hcp-FeH$_x$ transformed into fcc-FeH$_x$ at \~70$\text{ GPa}$. The compression behavior of fcc-FeH$_x$ was also obtained at 26 to 137 GPa. The pressure-volume relations and the compressivity showed an almost discontinuous change at \~70$\text{ GPa}$, which may reflect the magnetic transition of fcc-FeH$_x$, as indicated by theoretical calculations in Isaev et al., 2007. According to these results, the structure of FeH$_x$ at core conditions of the Earth may be fcc rather than dhcp.

Keywords: core, hydrogen, fcc structure, high pressure, X-ray diffraction
Sound velocities of liquid Fe-Si alloys at 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 on the Earth’s core condition by dynamic techniques using explosive [5], gas gun [5, 6], and laser [7]. However, the previous dynamic compression experiments are not enough to reveal the core of Earth, giant planets [8], and super-Earth which is at core pressures over 800 GPa [9]. In this study, we measure the sound velocity and density of liquid iron alloys by shock-compression method using high-power laser at pressures corresponding to super-Earth core pressures.

We conducted shock-compression experiments using a High Intensity Plasma Experimental Research (HIPER) system at the GEKKO-XII laser irradiation facility [10] at the Institute of Laser Engineering, Osaka University. The samples are Fe-Si alloys (Fe$_{95}$Si$_5$, Fe$_{90}$Si$_{10}$, Fe$_{80}$Si$_{20}$, and Fe$_{66}$Si$_{34}$ in weight percent). The sound velocities and densities of shock-compressed Fe-Si alloys using the high-power laser were measured by x-ray radiography [7, 11, 12] at pressures up to 960 GPa. The linear relation between the sound velocity and the density for FeSi alloy well follows Birch’s law [4] up to 960 GPa along the Hugoniot. The extrapolated sound velocity of FeSi alloy was about 40% faster than that of PREM at inner core boundary pressure. The outer core is composed of Fe-Si alloy with 5-13 wt.% Si assuming Si is only light element at the core. This Si content is consistent with the results of previous work by sound velocity measurement [13] and shock-compression experiment [14].

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References

Keywords: sound velocity, laser, shock wave, Fe-Si alloys, Earth’s core, experiment
The liquid Earth’s outer core is composed mainly of iron (Fe)-nickel (Ni) alloy. Birch (1952) first found that the core is less dense than pure iron based on comparison between seismological observations and experimental measurements of the density of solid iron. This is the so called “core density deficit” problem. He suggested the existence of lighter component(s) in the core, and hydrogen (H), carbon (C), nitrogen (N), oxygen (O), silicon (Si), and sulfur (S) have been identified as likely candidates from cosmochemical and geochemical arguments (e.g., Poirier et al., 1994). The density difference between the outer core and the pure iron has been estimated to be 5-10%, depending on the assumed outer core geotherm (e.g., Anderson and Isaak, 2002). The nature of light elements has remained one of the biggest enigmas for the more than half-century since the Birch’s work (1952). To justify the kind and quantity of the light elements in the core, sound velocity measurements of liquid iron alloying with possible lighter elements are fundamental because they link directly to seismological observations. We have launched the project on the sound velocity measurements for liquid iron alloys at high pressure in externally-heated and laser-heated diamond-anvil cells (DAC). The sound velocity of liquid (Fe,Ni)\textsubscript{3}S was measured via a high resolution inelastic X-ray scattering (IXS) measurements at BL35XU of the SPring-8 synchrotron facility, Japan (Baron et al, 2001). We successfully determined the sound velocity of liquid (Fe,Ni)\textsubscript{3}S up to the pressure of 50 GPa, which corresponds to the center of Mars. With our newly obtained results, we discuss the possibility of sulfur in the liquid cores of Earth and Mars.

Keywords: Sound velocity, liquid iron alloy, sulfur, outer core, Martian core
Earth’s outer core composition constrained by ab initio thermoelasticites of liquid Fe alloys

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The density deficit of the Earth’s outer core indicates substantial amounts of light elements (O, Si, S, C, and H) incorporated in the outer core (Birch, 1952; 1964). The chemistry and amount of the light elements have been strongly debated for over 60 years. Ab initio molecular dynamics (AIMD) simulations have been widely applied to investigate several properties of liquid Fe and Fe alloys (e.g., Alfe et al., 2002; 2007; Badro et al., 2014; Ichikawa et al., 2014). Badro et al. (2014) recently reported a likely compositional model being consistent with seismological data. However with applying empirical pressure corrections, the model suggests smaller amount of light elements to reproduce the ICB density jump. In our study, adopting the Ichikawa et al. (2014) technique we determined the equations of state (EoS) of the liquid Fe alloys by means of the AIMD method in the P, T condition widely covering the entire outer core condition without any pressure corrections. From the EoS, densities, adiabatic bulk moduli, and finally P-wave velocities were calculated and compared with the seismological data (PREM) (Dziewonski and Anderson, 1981). After examining alloy systems from binary to quaternary, we could find some optimized compositional models. However, these have almost comparable reproducibility to PREM, suggesting that other observables are required to make further constraints on the outer core composition. If considering the observed large ICB density jump additionally, Fe-Ni-Si-O and Fe-Ni-S-O compositions appear the most likely.

Keywords: Earth’s outer core compositional models, Ab initio molecular dynamics simulations, Equation of state of liquid Fe alloys
Fine seismic velocity structure of the lowermost outer core determined using outer core sensitive phases

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The liquid outer core of the Earth is regarded as homogeneous and approximately in hydrostatic equilibrium [Stevenson, 1987]. However, a low-velocity layer appears at the base of the outer core (F-layer) [Souriau and Poupinet, 1991; Kennett et al., 1995]. This basal layer may exhibit hemispherical features, as reported by Yu et al. [2005], corresponding to the quasi-hemispherical pattern of the inner core [Tanaka and Hamaguchi, 1997; Wen and Niu, 2002]. The pattern of the inner core is suggested to reflect solidification and melting at the inner core boundary (ICB), which might cause an Fe-rich or Fe-poor layer in the F-layer [Gubbins et al., 2008; Alboussiere et al., 2010; Monnereau et al., 2010]. However, the seismic profile of the F-layer is poorly revealed because of the non-uniqueness of the profiles investigated using previous methods and the interdependence of the F-layer velocity and other seismic properties of the Earth. Thus, a better constrained F-layer velocity is required before discussing its composition.

In this study, we investigated the velocity profile of the F-layer using two new methods: frequency dispersion of the traveltimes of waves that graze or are diffracted at the ICB, and differential traveltimes between waves reflected from the boundary and those that turn above the boundary. The first approach is sensitive to velocity gradients in the layer, while the second is sensitive to velocity excesses or deficits relative to a reference model for the layer; neither approach is sensitive to inner core properties or its radius. We analyzed seismograms of South American earthquakes observed using the Hi-net array [Okada et al., 2004] and the J-array network [J-Array Group, 1993] in Japan. The area investigated in the study is beneath the eastern Pacific, which is placed on the quasi-western hemisphere of the inner core.

Our results show that Vp values in the F-layer are intermediate between those of AK135 and PREM, and that the vertical velocity gradient is larger than that of AK135. Nearly constant velocities in the F-layer are not suited to observations.

Keywords: P-wave velocity in the lowermost outer core, F-layer, Traveltime dispersion of PKPbc, differential traveltimes between PKiKP and PKPbc

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Plate tectonics plays a role of global material circulation from the surface of the earth to the bottom of mantle since ca.4.0Ga. This is a due function both to bear habitable planet and to evolve as a habitable planet.

In spite of empirical recognition of importance of plate tectonics, nobody succeeded to synthesize the role of plate tectonics. However, the author completed this task by using following data; (1) geophysical constraints for the mechanism of plate tectonics, (2) petrological and geochemical characteristics of lithosphere, and (3) geologic history of the Earth, specifically the structural and petrological remarks of rock components and dynamics recorded in orogenic belts over the world.

As the result, basic condition for the operation of plate tectonics and following 6 roles of plate tectonics were summarized. The reason why plate tectonics is operated on the Earth is because mid-oceanic ridge is hydrated to enable plate to subduct which is helped by the lubricant water-rich fluids on the bottom of lithosphere. Roles of plate tectonics are (1) Global material circulation of CO2 and H2O, (2) Role of tectonic erosion, (3) Production of nutrients-source rocks at subduction zone, (4) Driving force of Earth’s magnetic filed, (5) The buffer of Earth’s system, and (6) The controller of thermal history of the Earth.
East-west hemispherical structures in the Earth and their implications for global dynamics

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Hemispherical structures have been found in the inner core (Tanaka and Hamaguchi, 1997; Waszek et al., 2011; and the references therein), the outer core (Tanaka and Hamaguchi, 1993; Yu et al., 2005), and the mantle (Iwamori and Nakamura, 2012). While seismic velocities characterize the core hemispherical structures, the mantle east-west hemispheres have been proposed based on geochemistry, rather than south-north division as has been long argued for (Hart, 1984, known as “Dupal anomaly”). In order to better characterize and interpret the mantle geochemical hemispheres in both spatial and compositional domains, and to discuss whether the hemispherical structures in the core and mantle have any dynamical linkage or not, a total of 6854 young basalt data consisting of five isotopic ratios of Sr, Nd and Pb from almost all tectonic settings (mid-ocean ridge, ocean island, arc and continent) have been statistically analyzed (Iwamori and Nakamura, 2015).

As a result, it has been found that the continental basalts are mostly distributed only in the eastern hemisphere, while other basalts are distributed evenly. Using multivariate analysis (Independent Component Analysis, ICA), two independent compositional vectors have been extracted, which explain most of the sample variance (95%). Therefore, almost all young basalts from various tectonic settings plot on a single isotopic compositional plane, and can be explained solely by two elemental differentiation processes (e.g., melting and aqueous fluid-rock interaction, Iwamori and Albarede, 2008). One of the independent components (IC2) represents ‘anciently subducted aqueous fluid component’ stored for 300 to 900 million years in the mantle, and defines the fluid component-rich (=positive IC2) eastern hemisphere, while the western hemisphere shows the opposite polarity. We have also found a striking geometrical similarity between the IC2 and the inner core hemispheric structures (Iwamori and Nakamura, 2015): the eastern hemisphere shows positive IC2 in the mantle and high seismic velocities in the inner core. Combining these constraints, we propose ‘top-down hemispherical dynamics’: focused subduction within and around the supercontinent has created a fluid component-rich hemisphere with a lower temperature, compared to the oceanic mantle. The colder hemisphere seems to have been anchored to the asthenosphere during the continental dispersal, and may affect the temperature and growth rate of the inner core, resulting in the coupled hemispherical structures in the mantle and the core.

Keywords: mantle, core, supercontinent, hemispherical structure, isotope, independent component analysis
Slab dynamics and water transport in the lower mantle

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Cold and dense subducting slabs characterize Earth’s mantle convection. The structure and evolution of the lower mantle must be significantly influenced from the lower mantle slab, as seismic tomographic images indicate that the slabs penetrate into the lower mantle. For example, the morphology of the large low shear velocity provinces (LLSVPs) at the base of the lower mantle (Romanowicz, 2003) and distribution of a fluid mobile component show the relationship with the subduction history (Iwamori and Nakamura, 2012). We perform a numerical study to investigate influences of the lower mantle properties on the mechanical interactions of the subducted slab with the lower mantle structure.

We use a 2-D Cartesian model of the mantle convection system in which plate-like motion is realized without any imposed forces. We incorporate hydrous mineral phase diagrams (Iwamori, 2004, 2007) and water transport into the model. A chemically dense layer and a post-perovskite (PPV) phase change are introduced to examine interaction between the subducted slab and the D” layer. We also consider effects of various depth dependence of viscosity and a thermal expansivity. Furthermore, yield strengths of the slab are varied.

In the cases with the slab yield strength of 200 MPa except when the lowermost mantle viscosity is as small as $10^{22}$ Pa s, the subducted slabs experience buckling. By introducing the thermal expansivity declining with the depth, the slab buckling occurs even when the slab yield strength is 300 MPa. The reason of this is that the depth dependence of the thermal expansivity decreases the slab negative buoyancy in the deeper mantle. On the other hand, the depth-dependent thermal expansivity promotes the subduction of the lithosphere, because of the larger value of the thermal expansion coefficient than that for the constant case in the shallow mantle. Accordingly, the plate motion at the surface is less affected by the slab behavior in the lower mantle. The wavelength and the slab descent rate depend on the viscosity profile.

The slab viscosity in the lowermost mantle also influences segregation of the slab materials in the CMB region. In the case with small lowermost mantle viscosity, the slab descends as fast as 20 cm/yr. The rapid slab collision with CMB generates a kink of the slab above the CMB. This reduces the viscosity of the slab by means of the yielding. This causes that a hydrated layer in the upper-side of the slab tends to be segregated from the slab. The hydrated materials are distributed to the overriding-plate side of the slab. When the slab sluggishly descends in the CMB region, the hydrated layer is not peeled. Even in this case, introduction of the viscosity reduction due to the PPV phase transition induces the hydrated slab layer segregation.

In summary, the yield strength and the thermal expansivity play a key role to control the slab-lower mantle interaction. We also emphasize that the viscosity of the PPV phase affects water transport in the lowermost mantle.

Keywords: free convection, subducting slab, slab buckling, lower mantle structure, water transport
Mapping the North American continent with inter-station phase and amplitude data of surface waves

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The investigation of a three-dimensional upper mantle structure using seismic surface waves has been generally based on the measurements of phase delay. The lateral heterogeneity in the Earth, however, not only affects the phase of surface waves, but also modulates their amplitude through focusing/defocusing effects. Such amplitude anomalies caused by elastic focusing are dependent on the second derivative of phase velocity across the ray path, and thus they are sensitive to short-wavelength structure than the conventional phase data, which should be useful for improving the lateral resolution of phase velocity models. In this study, we collect a large-number of inter-station phase velocity and amplitude ratio data working with a non-linear waveform fitting technique using USArray seismograms. Phase velocity maps of North America are then constructed using both phase and amplitude data of both Rayleigh and Love waves to check the validity and utility of inter-station amplitude measurements for enhancing the quality of the phase velocity models.

The phase velocity maps derived only from phase data reflect large-scale tectonic features well; e.g., slow anomalies in the tectonically active western U.S. and fast anomalies in the eastern cratonic region. To the contrary, phase speed models derived from amplitude data tend to emphasize smaller-scale structures characterized by strong lateral velocity gradients; e.g., significant slow anomalies in Snake River Plain and Rio Grande Rift, where the local amplification due to elastic focusing has been observed at USArray stations. Our results indicate that inter-station amplitude-ratio data reflect the effects of the second derivatives of phase velocity distribution well, and are extremely useful for reconstructing shorter-wavelength elastic structures. Thus, the measurements of inter-station amplitude ratios across a dense seismic array can be used to enhance the horizontal resolution of phase velocity models of surface waves.

Keywords: surface wave, phase velocity, amplitude, tomography, North America
Detection of an asthenospheric thermal event: approach from lithospheric mantle xenoliths

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Convective mantle heat flux through the continental lithosphere is not well constrained because of high heat generation in the overlying continental crust (Sclater et al., 1980; Pollack et al., 1993; Jaupart et al., 2007; Jaupart and Mareschal, 2007). Its proper estimation and its temporal variation through the earth’s history is important to know the overall rate of heat loss from the convecting interior of the earth (Labrosse and Jaupart, 2007; Korenaga, 2008), although the earth is thought to be losing most of its internal heat through the oceanic lithosphere (70%; Jaupart et al., 2007; Mareschal et al., 2012). The sub-continental lithosphere-asthenosphere boundary (LAB) is the interface through which entropy transported to the asthenosphere beneath the LAB via mantle convection from the depth of the earth is passed on to the entropy transfer in either steady or transient state through the sub-continental lithosphere (Jaupart and Mareschal, 2007; Michaut and Jaupart, 2007; transient important). There are three important mechanisms of entropy transfer through the LAB: heat conduction, solid-state flow, and magmatism (Jaupart and Mareschal, 2007). The uppermost zone of the asthenosphere acts as the upper thermal boundary layer of the convecting mantle and that the heat was transferred via heat conduction in the continental lithosphere with or without LAB modification (thickening or delamination/thermal erosion of the lithosphere; Moore et al., 1999; Jurine et al., 2005). Another important aspect of the sub-continental LAB is that it roughly corresponds to a boundary where melting and segregation of melt take place either via decompressional melting in the asthenosphere or melting of the lithospheric mantle induced by the heat input or material influx. This implies that entropy can be transferred from the convecting interior to the lithosphere via magmatism involving heat release or absorption by melting, crystallization, and open-system reactions. It is important to know where magmas are generated and crystallized during its ascent to the earth’s surface in the continental region in order to evaluate the role of magmatism in heat transfer through the sub-continental LAB. If a magma generated in the asthenosphere releases heat directly on the earth’s surface ending as volcanic eruption and intrusion, then heat loss via magmatism is at maximum efficiency (Ogawa, 1988). Contrary to this, if the magma releases heat within the lithosphere or crust by freezing all the melt there, it heat up the host layer. In this case, the enhancement of heat loss via magmatism depends on the depth of magma freezing, though it is higher than exclusively conductive heat transfer.

In order to examine heat transfer near the sub-continental LAB, it is important to scrutinize the thermal state and its temporal and spatial variability of the mantle material near the LAB and concomitant magma formation and its subsequent magmatism. Fortunately, we have many samples from the continental lithosphere as mantle xenoliths, though xenoliths from the asthenosphere are limited. The continental lithospheric mantle has long history of its formation and modification, but we can extract not only thermal records when xenoliths were entrapped by erupted magmas (mantle geotherm) but also their temporal change before the entrapment by carefully looking at reaction processes took place responding to various thermal and chemical changes taking place in the vicinity of the LAB.

Keywords: asthenosphere, lithosphere, thermal event, mantle xenolith, mineral zoning
An alternative formulation of the dynamics equation system of Maxwellian viscoelastic media

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The traditional dynamics equation system for Maxwellian viscoelastic media is re-examined to find an alternative form which has clearer and sounder physical basis. In the alternative formulation, in the equation of motion only elastic stress should be considered regardless of time scales, while the constitutive equation should be rewritten into such an alternative form that expresses transformation of elastic strain into permanent (plastic) strain with a time constant of the Maxwell relaxation time. Generally for long time scale phenomena, the equation system expresses gradual transformation of elastic strain into permanent strain by always keeping quasi-elastostatic balanced state. Particularly in incompressible case, the system becomes mathematically equivalent with the equation of viscous fluid motion, if the changing rate of elastic to permanent displacement is identified with fluid velocity. Practical method to time-integrate the equation system is investigated. Guided by the new formulation and underlying conception questionable points in traditional treatments of geophysical dynamics are discussed.

Keywords: plate-mantle coupled system dynamics, mantle convection, Maxwellian viscoelastic medium, viscoelastic medium dynamics, elastico-plastic medium dynamics
The boundary mode of axially symmetric MAC waves can exist in the stratified layer at the top of the Earth’s outer core

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Seismological observations (e.g. Helffrich & Kaneshima(2010), Kaneshima & Helffrich(2013) ) and theoretical predictions show the existence of a layer stratified by the accumulation of light fluid at the top of the Earth’s outer core. Helffrich(2014) suggested that its most probable origin is the vestige of primitive Earth. MAC waves, which arise from the balance among magnetic, Archimedes and Coriolis forces, can exist in the stratified layer. To explain the cause of the 60-year variations of the geomagnetic field, Braginsky(1993) examined axially symmetric approximate solutions of MAC waves theoretically. In his model, a boundary exists, where the fluid density is discontinuous between the layer and the bulk of outer core, and the buoyancy frequency is constant within the layer. (Recent seismological observations, however, indicate that the density jump is unlikely at the boundary.) The latitudinal phase velocity of the solution is equal to the Alfvén wave velocity multiplied by the buoyancy parameter (\(c_{lat} = V_A \cdot B_u = V_A \cdot N / f\), where \(c_{lat}\) is the latitudinal phase velocity, \(V_A\) is the Alfvén wave velocity, \(B_u\) is the buoyancy parameter, \(N\) is the buoyancy frequency, and \(f\) is the Coriolis parameter), and the vertical structure is expressed as a superposition of sine waves. The decay rates of the wave are proportional to the magnetic diffusivity. Since the latitudinal phase velocity is proportional to buoyancy frequency, the stratification can be estimated if the phase velocity is determined observationally. If the 60-year variation of the geomagnetic field is identified as the fundamental mode with the latitudinal wavenumber \(l=2\), the buoyancy frequency is estimated to be about twice the angular velocity of the Earth’s rotation.

We have found that Braginsky’s(1993) equations also have the solutions localized at the layer boundary, which we refer to as the boundary mode. This mode has a time scale smaller than the solution within the layer (Braginsky’s(1993) solution), and spreads through magnetic diffusion. The phase propagates away from the layer boundary. The frequency of the boundary mode does not depend on the buoyancy frequency within the layer. The frequency and the vertical wavenumber depend on the magnitude of the density discontinuity, the latitudinal wavenumber, and several parameters. The wave amplitude decreases exponentially with the distance from the layer boundary. As the density jump or the latitudinal wavenumber increases, temporal and spatial decay rates increase. Therefore, small density jumps and small layer thicknesses are required to find the boundary mode observationally, and waves with smaller latitudinal wavenumbers are expected to be observed more easily. If the 60-year fluctuation of the geomagnetic field is identified as the boundary mode with the latitudinal wavenumber \(l = 2\), the ratio of density discontinuity is estimated to be about \(10^{-4}\). Furthermore, the boundary in contrast to the MAC wave within the layer, the spatial and temporal decay rate of the boundary mode decreases as the magnetic diffusivity increases.

Keywords: MAC waves, the top of the Earth’s outer core, H layer
Effect of sulfur on the reaction between iron and water under high pressure and temperature

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It is reported that hydride phase such as FeH and FeOOH appears by a reaction between Fe and H\(_2\)O under the Earth’s deep environment during the formation stage (e.g., Okuchi, 1997; Ohtani et al., 2005). In this study, we added sulfur and observed a reaction of the Fe-S-O-H system under high pressure and high temperature to investigate the effect of sulfur on Fe-O-H system.

Because hydrogen in metal hydride, which is expected to produce in the reaction, is dissipated from the sample at low pressure, we carried out the experiments at High Energy Accelerator Research Organization (KEK), Photon factory (PF-AR-NE1A), and identified phase transitions of the sample and the reaction products by in situ X-ray diffraction method.

We used a laser-heated diamond anvil cell installed at AR-NE1 to generate high pressure and high temperature. Starting materials were pelleted FeS and pure water in rhenium gasket. The pressure was measured using the equation of state of ice V\(\text{II}\). The double-sided heating with Nd:YAG laser to heat, the reaction temperature was estimated from radiation of the high temperature portion of the sample.

In this study, the pressure was 24 and 33 GPa and the temperature was between 300 and 1200 K. As a result, FeS\(_2\) (Pyrite), dhcp-FeH\(_X\) and \(\epsilon\)-FeOOH appeared as the reaction product. It was revealed that stability field of \(\epsilon\)-FeOOH is much higher pressure than that of Fe-O-H system, high temperature decomposition of \(\epsilon\)-FeOOH was also constrained, FeS\(_2\) which doesn’t appear in the Fe-S-H system is observed. We will present further result of SEM-EDS analysis of the recovery sample.

Keywords: Earth’s core, light element, hydrogen, synchrotron
Measurement of thermal conductivity of mantle minerals at pressures of the transition zone to the lower mantle

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Knowledge of thermal diffusivity or thermal conductivity of the mantle is vital for study of the dynamics of the Earth. So far we have measured thermal diffusivity and thermal conductivity of upper mantle minerals, i.e. olivine and garnet and hydrous phases, i.e. serpentine and talc. All those data were obtained by the experiments at pressures up to 10 GPa and temperatures to 1100 K. The measurements were conducted by a pulse-heating method of one-dimensional heat flow using the Kawai-type apparatus at the Institute for study of the Earth’s interior, Misasa. This current method is a predominant one for study in deep Earth’s materials under pressure. It has some advantages as follows: (1) comparatively small amount of samples (2) applicable to materials with anisotropy in thermal conduction (3) simple cell assembly. Moreover, this method enables to obtain specific heat capacity under pressure.

In order to expand pressure range the cell assembly is needed to advance by reducing its dimensions. A new cell-assembly similar to our previous one is designed for a sample of 2.6 mm in diameter and 0.6 mm in thickness. This smaller cell is installed in a 14 mm edged octahedral pressure medium in 7 mm truncated anvils. This cell enables to make measurements of the thermal properties at pressures exceeding 15 GPa, which will covers the condition in the mantle transition zone. The cell will be also applied to pyroxene samples of which sizes are necessarily limited. Test measurements were made using garnet samples. The results agree well with those of the previous experiments using the larger (18-11 and 14-8) cell, and the extrapolations to zero-pressure coincide to values of other methods. Thus, the pulse heating method will be applied for thermal property measurements of wadsleyite, ringwoodite and majorite. Using large anvils ( >46 mm), the method is probable to measure the thermal conductivity of MgSiO₃ perovskite (bridgmanite). However, measurements at high temperature still have somewhat problems in precision. Materials of impulse heater and external furnace should be re-considered. The precision of measurements should be improved by well-controlled machining of the cell assembly and by refining the data acquisition system.

Keywords: mantle minerals, thermal diffusivity, thermal conductivity, high-pressure, Kawai-type apparatus
Lattice diffusion in MgO crystal from first principles simulation

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Rheological property is critical to understanding the mantle convection. Diffusion creep might be the dominant deformation mechanism in the Earth’s lower mantle and super-Earths’ mantle (e.g., Karato, 2011). Thus several experimental and theoretical studies have tried to measure lattice diffusion coefficients under pressure, which are both still technically difficult. There are two theoretical approaches to calculate self-diffusion coefficient in solids. One is based on the static lattice energy calculation and the other is based on the molecular dynamics simulation. In the former case, it is difficult to evaluate attempt frequency and in the latter case, atoms are hardly mobile in actual computation time at the Earth’s lower mantle and super-Earths’ mantle temperatures. These two approaches were previously applied to MgO, one of major deep mantle constituents (Ita & Cohen, 1997; Ito & Toriumi, 2007). However reported pressure dependences of the self-diffusion coefficients are contradictory with each other particularly at high pressure over 80 GPa.

In this study, we develop a new theoretical method to calculate self-diffusion coefficient in crystals with charged vacancies (Schottky pair) within the first principles framework. This method was then applied to NaCl-type MgO. We found that the calculated pressure dependences of the self-diffusion coefficients in MgO are consistent with those of Ita & Cohen (1997). Diffusion creep viscosity of MgO was then estimated using calculated diffusion coefficients. Our activation volumes are consistent with experimental values at low pressure (Van Orman et al., 2003) and decrease rapidly with increasing pressure. It suggests that super-Earths’ mantle would not be quite viscous and the constant activation volume extrapolation leads to overestimation of viscosity in the deep mantle.

This method is widely applicable to other materials including bridgmanite, post-perovskite and CsCl-type MgO, which are important to analyze more realistic planetary interior dynamics.

Keywords: MgO, lattice diffusion, Earth’s lower mantle, super-Earths’ mantle, first principles
Are LLSVPs formed in the Earth’s lowermost mantle by the subduction of oceanic crusts?

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We conducted a series of numerical experiments of thermo-chemical mantle convection where a subduction is preferentially induced at a continental margin, in order to verify a hypothesis that the Large Low-Shear Velocity Provinces (LLSVPs) in the Earth’s lowermost mantle are formed by subduction of oceanic crust. In this study, we adopted a model of two-dimensional rectangular box of 2900km height and aspect ratio 6 with reflective boundary condition in the horizontal direction. We placed an immobile lid as a model of surface supercontinent which covers a third of the top surface. We also put a thin layer of chemically dense materials as a model of oceanic crust, which may sink into the deep mantle along with cold descending flows from the top surface.

Our calculations showed that the subducted oceanic crusts are preferentially provided under the continent when the subduction at the margin of continent is stable. However, stable subduction caused strong convection and significantly stirred the mantle under the continent. Therefore, subducted oceanic crusts were distributed almost uniformly under the continent without accumulating on the CMB. On the other hand, the cases with unstable subduction at the margin of continent showed a long-wavelength mantle convection structure which has an ascending plume along the side wall under the continent and a descending plume at the opposite side wall. The large-scale flow gathered subducted oceanic crusts under the continent and formed large piles on the CMB.

Our results suggest that the LLSVPs are hardly formed in the presence of stable plate tectonics like the current one where a stable plate motion including subduction stirs the mantle very effectively. In other words, the formation of large thermochemical piles which are equivalent to the LLSVPs should have been completed before the plate tectonics is well established, assuming that subducted oceanic crusts are the origin of LLSVPs.

Keywords: mantle convection, numerical simulation, LLSVP, plate subduction
Experimental presentation of plate subduction using paraffin wax

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Experimental approaches using analogue materials have been widely used to understand kinematic behaviors of tectonic plates. Previously molten paraffin in a tank inside a hot water bath has been used. Although tectonic plate-like behaviors, such as inclined subduction and trench migration, have been observed, the “plate” in this case was too thin to reproduce the lithospheric strength and the heat balance through the thermal boundary layer of the Earth. In order to simulate the plate and its motion as a well-developed thermo-mechanical boundary layer on top of vigorously convecting mantle, we have developed a tank apparatus and performed preliminary experiments using paraffin wax.

To control the complex heat and convection processes and for easy observation we constructed a glass tank with an inner size 120x23x4cm. The walls are constructed from double pane glass with panes separated by air gap to reduce heat loss, and reinforced with aluminum plates and bars. The paraffin was melted from bellow by a copper heat-sink containing 24 ceramic heating elements. To reduce heat loss to the back wall, the wall was isolated with 8cm thick foam. At the boundary layer where the paraffin wax was sticking as it cooled down we applied NiCr wire heater to the inner walls. All heating sections were controlled by variable controllers. We cooled the top layer of the wax with a cold air flow carefully controlled with thin foam plates from a vat filed with liquid Nitrogen.

The biggest challenge was the “frosting” effect especially on the front uninsulated wall that prevented the “subduction” of the forming “crust” to deeper levels. External wall temperature was 65 °C, 70 °C was measured at the boundary level by the wire heater, while the wax inside the tank was at 80 °C. Some external force was necessary to initiate a start of subduction. The maintenance of balance between the various heaters, the wall temperature, the wax temperature and the cooling rate was critical for the successful completion of the experiment.

We observed continuous subduction and clear “crust” forming with subsequent “subduction”. We can say that our experiment properly reproduces the general features of plate motion of the earth. Artificially fracturing or weakening the boundary layer and applying a vertical, downward external force were required to initiate subduction in addition to collision of the plates. The thickness of the plate was the primary parameter controlling subduction behavior and plate motion. The plate showed elastic and plastic behavior depending on its thickness and temperature. A cold and thick “plate” did not subduct even after applying an external force, and formed a stagnant lid. A hot and thinner “plate” did not show continuous subduction behavior, plate motion stopped soon after subduction was initiated, possibly because the slab pull force from the thinner partially subducted slab was too weak. Our experiment results suggest that the driving force of subduction and plate motion is slab pull, not the thermal convection of the molten paraffin or ridge push. We will present photos and videos of the observed processes.

Improvements to the tank and heating elements design are necessary to provide better and easier control over the experiments.

Keywords: analogue experiment, plate subduction, paraffin wax, glass walls tank, slab pull
Numerical experiments on mantle convection of super-Earths with variable thermal conductivity and adiabatic compression

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Recently, many extra-solar planets have been discovered by improved observation technologies. Some of these planets, called super-Earths, have small masses (up to 17 times the Earth’s) and high mean density (>5000 kg/m³). Numerical modeling of mantle convection of super-Earths plays an important role in studying the occurrence of plate tectonics and the surface environments on these planets. On the other hand, when considering mantle convection of super-Earths, it is also important to take into account the difference in (hydrostatic) pressure in the mantles. Since super-Earths have high inner pressure, there must exist a strong change in physical properties and the effect of adiabatic compression. While the effects of physical properties have been intensively studied so far, those of adiabatic compression have not been well studied in the previous models of mantle convection of super-Earths. Here we conduct numerical experiments of thermal convection of highly compressible fluid in a two-dimensional rectangular box whose thermal expansivity and conductivity are dependent on depth, viscosity is dependent on temperature, in order to elucidate the mantle convection on super-Earths.

Our numerical experiments showed the change in convecting flow patterns depending on the temperature-dependence in viscosity, regardless of the depth-dependence in thermal conductivity. When a viscosity is sufficiently dependent on temperature, horizontal flow becomes dominant in the mantle, with a very weak activity of hot plumes from the base of the mantle. This flow pattern is quite similar to the ”stratosphere” in the field of meteorology. In addition, we found that the occurrence of ”stratosphere” is enhanced for a strong depth-dependent thermal conductivity. One reason for this is that high conductivity at depth significantly reduces the difference in temperature between the basal thermal boundary layer and isothermal core. Our study therefore suggests that the depth-dependent thermal conductivity is one of the most important agents which control the mantle dynamics of super-Earths.

Keywords: super-Earths, mantle convection, adiabatic compression, thermal expansivity, thermal conductivity, viscosity
Implicit solution of the material transport of the core formation simulation

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In order to investigate the long time-scales of the global core formation process in a growing planet, we are developing the Stokes flow simulation code using MIC based techniques for material transport with a free-surface treatment. We are interested in the dynamical change of the internal structure after solidification of magma ponds/oceans during the core formation under a self-gravitating field, especially because it might lead to an initial heterogeneous structure in the deep mantle.

However current numerical solution method is difficult to solve the system coupled with the energy equation because the numerical system becomes stiff when the dynamical balancing time scale for the increasing/decreasing load by surface deformation is very short compared with the time scale associated with thermal convection. Any explicit time integration scheme will require very small time steps; otherwise, serious numerical oscillation (spurious solutions) will occur.

In this work, we propose to treat the advection as a coordinate nonlinearity, coupled to the momentum equation, thereby defining a fully implicit time integration scheme suitable for stiff problems [Furuichi and May, Compt. Phys. Commun 2015]. We utilize a Jacobian free Newton Krylov (JFNK) based Newton framework to solve the resulting nonlinear equations. We also investigate efficient solution strategies to reduce the computational cost to evaluate the nonlinearity on MIC advection.

These implicit methods are implemented within FD framework [Gerya and Yuen, 2003]. We examine the solution quality and efficiency of these methods by performing numerical experiments we have performed a series of numerical experiments which clarify the accuracy of solutions and trade-off between the computational cost associated with the nonlinear solver and time step size.

Keywords: core formation, Stokes flow, free surface, implicit time integration, JFNK
Modeling of SKS splitting parameters measured in Japan with Hi-net

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To systematically investigate the spatial variation of seismic anisotropy around Japanese islands, we measured splitting parameters (fast polarization direction $\phi$, delay time $\delta t$) of teleseismic SKS phases observed by Hi-net (Ogawa et al., 2014, SSJ). The results indicated regional scale variations of splitting parameters that are apparently related to subduction systems. In order to investigate detailed anisotropic structures (fabric in mantle wedge, subducting slab, and asthenosphere), we conducted forward modeling using synthetic seismograms. We modeled the SKS phases by the ray theory. We assumed that the SKS ray is straight and that each region has homogenous anisotropy. We rigorously calculated the phase velocity in each region by solving the Christoffel matrix. The preliminary analysis indicates that the measured splitting parameters appear to be primarily affected by the A-type fabric in subducting slab (oceanic lithosphere) whose $a$-axis aligns in the direction of the fast axis observed at the surface by using our OBS data.

Keywords: seismic anisotropy, s-wave splitting, modeling
Constraining radial anisotropy in the upper mantle with multi-mode surface waves

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The radial anisotropy of shear waves represents the differences in the propagation speeds between vertically polarized shear waves (SV) and the horizontally polarized ones (SH), and can be a key to the understanding of the dynamic processes in the upper mantle. Seismic surface waves are the most powerful tool to determine the spatial distribution of the radial anisotropy. Some recent studies have revealed the existence of a layer with strong radial anisotropy (with SH > SV) beneath the lithosphere; e.g., under the Pacific plate (Nettles & Dziewonski, 2008, JGR) and the Australian continent (Yoshizawa, 2014, PEPI). This is, however, not always the case and there are also some studies on radial anisotropy that do not show such a clear layer with SH > SV beneath the lithosphere. These differences may be related to the differences in model parameterization.

For the inversions of multi-mode phase speeds of Rayleigh and Love waves for radial anisotropy of shear waves, we can use either set of model parameters for the representation of the anisotropic S velocity; i.e., (A) SV velocity (Vsv) and SH velocity (Vsh), or (B) SV velocity (Vsv) and radial anisotropic parameter $\xi = (Vsh/Vsv)^2$. The choice of model parameters for inversion is arbitrary, but, through synthetic experiments, we have confirmed that this difference causes non-negligible effects on the reconstruction of radial anisotropic properties of shear waves. This is mainly caused by the differences in the sensitivity kernels of Love-wave phase speeds to Vsv, Vsh and $\xi$.

For the set of parameters (B) [Vsv, $\xi$], Love waves always have the largest sensitivity to Vsv with suppressed sensitivity to $\xi$, and the kernel shapes for both Vsv and $\xi$ are nearly identical. On the other hand, for the parameterization with (A) [Vsv, Vsh], Love wave phase speeds are controlled primarily by the kernels for Vsh, which have the largest sensitivity to Love wave phase speeds with little influence from Vsv, which can be better (and independently) constrained by Rayleigh waves.

Such intrinsic differences in the sensitivities of surface waves can lead to the different results in the estimation of radial anisotropy. Our synthetic experiments suggest that the parameterization with [Vsv, Vsh] would be preferable particularly when the radial anisotropy with SH > SV is caused by anomalously slow SV velocity, which is consistent with the recent anisotropy models reported in the fast moving Pacific and Australian plates. We have also found that the strong dependence of the retrieved anisotropy on the initial model, when we use [Vsv, $\xi$] as model parameters.

Keywords: radial anisotropy, surface waves, upper mantle, lithosphere, asthenosphere
The Japan Islands are characterized by complex structure and tectonics caused by four plates which are interacting with each other. Many seismic tomography studies using local seismic data have been made to investigate the 3-D velocity structure beneath Japan. However, the study areas of the previous researches are limited to the shallow part, in the crust and shallow mantle, whereas the deep structure beneath Japan (a depth range of 200-700 km) is not well known. Investigation of the deep structure is very important for improving our understanding of the subducting slabs and mantle upwelling, as well as subduction dynamics.

In this work, we apply teleseismic tomography to relative travel-time residuals of teleseismic events to study the 3-D P- and S-wave velocity structure of the Japan subduction zone. Although there have been several studies using P-wave data so far (e.g., Zhao et al., 1994, 2012; Abdelwahed and Zhao, 2007), few studies using S-wave data have been conducted. Using both P- and S-wave data, we can determine not only the P- and S-wave velocity structures but also other physical parameters such as Poisson’s ratio, which are useful for better understanding the physical property of the mantle.

Part of the P-wave relative travel-time residuals used in this work were chosen from the data collected by the previous studies (Zhao et al., 1994, 2012; Abdelwahed and Zhao, 2007). We selected 130 teleseismic events from the previous data sets based on the following criteria: (1) The epicentral distances range from 30 to 100 degrees from central Japan; (2) Each event was recorded by over 100 seismic stations on the entire Japan Islands. In addition, we newly collected data from 38 teleseismic events so that the event distribution becomes more homogeneous. Thus, our data set contains 168 teleseismic events which generated ~60,000 P-wave arrivals. Our S-wave data set contains ~40,000 arrivals from 56 teleseismic events.

We also selected ~3,000 local shallow and deep earthquakes from the JMA Unified Catalog, each of which was recorded by over 100 seismic stations. We applied the tomographic method of Zhao et al. (1994, 2012) to invert the local and teleseismic data simultaneously.

Both of our P- and S-wave tomographic images show that low-velocity anomalies exist in the mantle wedge beneath the volcanic front and back-arc area, which reflect hot upwelling flow in the mantle wedge associated with slab dehydration. High-velocity anomalies are revealed, which reflect the subducting Pacific and Philippine Sea slabs where intermediate-depth and deep earthquakes are located. Beneath western Kyushu, dipping high-velocity anomalies are visible down to ~400 km depth in both P- and S-wave tomography, suggesting that the Philippine Sea slab has subducted aseismically down to the mantle transition zone depth. In addition to the P- and S-wave tomography, we will also present images of Poisson’s ratio and the R value (dlnVs/dlnVp), which provide additional information on physical properties of the Japan subduction zone.
Seismic evidence for a mantle plume beneath the Cape Verde hotspot

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The Cape Verde hotspot is located in the African plate, about 2000 km east of the nearest plate boundary. It is composed of a group of late Cenozoic oceanic islands resting on a broad bathymetric swell on mature (>110 Ma) oceanic lithosphere. This hotspot has a positive surface heat flow, high geoid anomaly, and long-term volcanism. The last known volcanic eruption occurred at Fogo volcano in 1995.

We determined P- and S-wave tomography of the upper mantle beneath the Cape Verde hotspot using arrival-time data measured precisely from three-component seismograms of 106 distant earthquakes recorded by a local seismic network. Our results show a prominent low-velocity anomaly imaged as a continuous column <100 km wide from the uppermost mantle down to about 500 km beneath Cape Verde, especially below the Fogo active volcano, which erupted in 1995. The low-velocity anomaly may reflect a hot mantle plume feeding the Cape Verde hotspot.

Keywords: Cape Verde, hotspot, mantle plume, seismic tomography, mantle transition zone