

## A new form of the dynamics equation of Maxwellian visco-elastic media

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Dynamical property of the earth's interior down to the core-mantle boundary has so far been considered to be a Maxwellian visco-elastic medium. It behaves as an elastic body for short time-scale phenomena, while on a very long time-scale it shows fluid-like behavior. So the Navier-Stokes equation for viscous fluids is considered to be appropriate for describing mantle convection, and numerical simulations have been made based on the equation.

As a phenomenon for which both elastic body property and viscous fluid property are essential post-glacial uplift has been discussed based on the constitutive equation proposed by Maxwell. However, so far most of studies apply Laplace transform to expressing time evolution, so it is not possible to treat this problem by use of finite difference method, just like general circulation models of atmosphere and oceans. Thus it is not possible to extend numerical simulation of mantle convection to include elastic property of the plate near the earth's surface.

With intention to overcome this difficulty to enable us to conduct numerical simulations of mantle-plate general circulation, a new formulation of dynamics equations for Maxwellian visco-elastic media is attempted in this study

Keywords: Maxwellian visco-elastic media, visco-elastic medium dynamics, mantle convection, plate-mantle coupling simulation

## Effects of Al content on water partitioning between Opx and Ol: Implications for lithosphere-asthenosphere boundary

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Most minerals in the Earth's upper mantle contain small amounts of hydrogen (i.e. "water"), structurally bound as hydroxyl. Water has an important influence on the behavior of rock system. This small amount of water has an important influence on the behaviours of rock systems. A large viscosity contrast of more than two orders of magnitude was detected at depths of 70 km to 100 km beneath ocean and was defined as the lithosphere-asthenosphere boundary [1]. The origin of the lithosphere-asthenosphere boundary remains an enigma. The water distribution in the Earth is critical to the nature of the boundary. For example, Mierdel et al. (2007)[2] indicated that a high water solubility in aluminous orthopyroxene among mantle geotherm in the Earth's upper mantle would effectively contribute to a stiffening of the lithosphere. Therefore, precise knowledge on the distribution of water among mantle minerals is very important for understanding the Earth's dynamics. The Earth's uppermost mantle is composed mainly of olivine (Ol), orthopyroxene (Opx), clinopyroxene (Cpx), spinel, and garnet. In particular, Ol accounts for a large proportion (60 vol.%) of the Earth's uppermost mantle. In addition, Opx, which contains significantly more water than does Ol in the mantle xenolith, is the second phase of the Earth's uppermost mantle. The FeO content in mantle Ol shows very limited variation in range, whereas the Al content of Opx in the Earth's upper mantle decreases significantly with increasing pressure [3] Therefore, the variation of Al content in mantle minerals can be important for the solubility of water in mantle minerals.

To investigate the partitioning coefficient of water between Opx and Ol ( $D_{(Opx/Ol)}$ ) under low-water concentrations (3 ~ 387 wt. ppm) similar to the Earth's mantle conditions, high-pressure experiments have been conducted at pressures of 1.5-6 GPa and a temperature of 1573 K. The experiments were performed with Kawai-type multi-anvil and piston-cylinder apparatus by using starting materials of natural Ol and synthetic Opx with various Al contents. The water contents were obtained with a vacuum type Fourier transform infrared spectrometer (Jasco: FT-IR6100, IRT5000). Water content of minerals was calculated based on Paterson's calibration [4]. IR-spectra of Ol and Al-bearing Opx in this study are similar to those obtained by high-pressure experiments [5] and natural rocks [6], respectively. It is believed that broad bands in IR spectra of natural Opx are due to effect of crystal distortion by large Al substitution. On the contrary, IR-spectra of Al-free Opx are not consistent with those reported by Rauch and Keppler (2002) [7] likely because of the large difference of water fugacity.  $D_{(Al-freeOpx/Ol)}$  is  $\sim 1$  at all pressure conditions. However, the water contents of Al-bearing Opx are significantly larger than those of Ol at the same conditions. In addition, the effect of Al concentration in Opx on  $D_{(Opx/Ol)}$  becomes larger with increasing pressure. The high Al content in Opx significantly increases  $D_{(Opx/Ol)}$  and the trend increases with increasing pressure.  $D_{(Opx/Ol)}$  drops sharply at the pressure at which the Al concentration of Opx becomes nearly 0 in the Earth's mantle conditions.

These results imply that viscosity of the upper mantle decreases sharply at depths deeper than those in which orthopyroxene contains no Al. The dramatic change of  $D_{(Opx/Ol)}$  may explain the lithosphere-asthenosphere boundary beneath oceans and continents.

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Keywords: water partitioning coefficient, olivine, orthopyroxene, viscosity, FT-IR, lithosphereasthenosphere

## Acoustic velocities of MgGeO<sub>3</sub> gel at high pressure by Brillouin scattering

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Properties of silicate melts are essential for understanding evolution and dynamic behavior of the Earth and terrestrial planets. In the shallow mantle melting processes the density contrast between melts and crystals is well studied, but studies on the deep melting near the core-mantle boundary are still limited due to technical difficulties. The studies of amorphous material, analogs of melt, at high pressure can provide valuable insights about melts in the deep mantle. The Brillouin scattering method is suitable for velocity measurements of amorphous materials. It has been suggested that the change in coordination in the melt or glass structure reflects to the change in acoustic velocity. Thus we conducted sound velocity measurement using the Brillouin scattering method in diamond anvil cell at high pressure. We report in situ high-pressure acoustic velocity measurements of MgGeO<sub>3</sub> gel, an analogue of the MgSiO<sub>3</sub> melt, revealing the gradual coordination change of Ge from four- to six at least up to 80 GPa. We will conduct experiments at higher pressure in order to confirm the possible Ge coordination change in the gel expected to exist in the terrestrial and extraterrestrial planets.

Keywords: sound velocity measurement, high-pressure experiment, mantle dynamics, silicate melts, super-Earth

## Measurement of differential P-wave travel time between two BBOBSs with Correction for crustal reverberation

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Seismic observations under the ocean are very important to investigate three-dimensional structure of the whole mantle. However, it is difficult to pick up arrival times of P-waves because noise level of broadband ocean bottom seismometer (BBOBS) is in general high in the period range more than 5 sec. Instead of picking arrival times, differential travel times between two BBOBSs have been measured by cross-correlating the waveforms at a period of around 10 sec or more (e.g. Toomey et al. 1998, Tanaka et al., 2009).

The resolution of P-wave tomography become high effectively by taking dispersion of P-wave travel time into account with the finite frequency theory (e.g. Obayashi et al. 2013 JpGU meeting), and its effect is expected to be significant under the ocean where the observations have been sparse. Obayashi et al. (2004) showed dispersion of PP is generated by interference of crustal reverberations under its bounce point. The reverberation under the station also affects a direct P-wave. Especially the effect of the seawater reverberation is significant.

Obayashi et al. (2013) proposed a method of correction for such reverberations to measure differential travel times between any two stations. In this method a waveform is convolved by the response calculated for the crustal structure under the other station.

We applied this method to the BBOBS array at French Polynesia. In the case of the measurement between a BBOBS and a island station, the waveforms of the two stations become similar each other after the correction, suggesting the correction is effective. We report the characteristics of the observed dispersions and the very first result of P-wave tomography using the new observations.

Keywords: crustal reverberation, broadband ocean bottom seismometer, tomography

## Small shear modulus of cubic CaSiO<sub>3</sub> perovskite

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Ca-perovskite (CaPv) is considered to be one of the most abundant minerals in the Earth's lower mantle (LM) and was suggested to have distinctly larger shear modulus than MgPv from static calculations and mean-field theory (Karki and Stixrude 1999; Stixrude et al. 2007). In this study the elasticity of cubic CaPv is reinvestigated using density functional constant-temperature first principles molecular dynamics simulations with strict calculation conditions. First, we computed the stable structure of CaPv and found that the cubic phase is more stable than the tetragonal and orthorhombic in the LM P,T condition. The thermal equation of state of CaPv was analyzed using the MD data set, which indicates its thermal properties including Gruneisen parameter quite similar to those of MgPv. Along the adiabatic temperature, CaPv was found to have higher density than the PREM and 12.5% iron-bearing MgPv. Next, we calculated elastic constants of cubic CaPv. Our new results clearly demonstrate that cubic CaPv does not have anomalously large shear modulus suggested by previous calculations with a small computation cell. This is because the cell applied in the previous studies is too small to allow the rotational phonon motion of SiO<sub>6</sub> octahedra related to the zone boundary optic phonon instability. Acoustic wave velocities were finally determined from the elastic moduli, indicating no significant differences in velocities between CaPv and iron-bearing MgPv.

Keywords: Ca-perovskite, elasticity, lower mantle, first principles

## Seismic Constraints on an Enstatite Chondrite Earth

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Recently, Javoy et al., EPSL, 2010 suggested the possibility that Earth had an initial enstatite chondrite composition due to their similar oxygen isotopes. Currently, the calculations of the bulk silicate Earth (BSE) are based on the assumption that the initial Earth began with a composition very close to that of a carbonaceous chondrite. Thus, it is necessary to evaluate whether the 1D seismic properties of the Earth are more consistent with an initial enstatite or chondritic composition. The BSE of an enstatite chondrite Earth (ECE) is different from that of a carbonaceous chondrite since the magnesium/silicon ratio is much lower for the former, resulting in a lower mantle that is almost devoid of Mg. Hence, the primitive lower mantle of an ECE consists mostly of iron-rich perovskite and pure silica. The seismic velocities of these phases are much slower than Mg-perovskite which, by itself, is faster than PREM (the slower MgO phase is necessary to match PREM velocities). However, the present-day lower mantle would be a mix of the primitive upper mantle (ie. pyrolite) and the Mg-depleted lower mantle. The latest mineral physics results are used to calculate possible 1-D seismic profiles of the Earth associated with these two scenarios and to compare with those observed for the Earth today.

## Thermal property modeling of the core-mantle boundary

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Lattice thermal conductivity of minerals under pressure and temperature is a key property to understanding dynamics and evolution of the Earth's interior. We recently established an efficient ab initio technique for calculating the thermal conductivity of silicate minerals with complex structure and chemistry (Dekura, Tsuchiya, Tsuchiya, PRL, 2013). Calculated lattice thermal conductivity of MgSiO<sub>3</sub> perovskite agreed satisfactorily with experimental values at room temperature, and post-perovskite was found to have thermal conductivity quite different from perovskite's, indicating that the D'' discontinuity is not only the phase transition boundary but also the conductivity boundary. Using the obtained results, we determine the effective conductivity of the lower mantle and estimate the energy flow across the core-mantle boundary (CMB). Our results demonstrate that the CMB heat flux could change significantly from place to place by reflecting temperature heterogeneity located atop the core. A large CMB heat flow recently suggested from the outer core side can be reconciled only by considering polycrystalline assemblages yielding high-thermal conductivity.

Keywords: First principles computation, Thermal conductivity, CMB heat flow

## Waveform inversion for localized 3-D seismic velocity structure in the lowermost mantle beneath the Western Pacific

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We infer 3-D localized shear velocity structure in the lowermost 400 km of the mantle at the western edge of the Pacific large low shear velocity province (LLSVP) by applying waveform inversion to transverse component body-wave waveforms from the F-net seismic array in Japan. Our dataset consists of relatively long period (12.5-200 s) broad-band seismic waveforms of Tonga-Fiji deep focus and intermediate deep earthquakes. We conduct several tests to confirm the robustness of the inversion results. We find two low velocity zones at the bottom of the target region, with a high velocity zone in the middle, and a low velocity zone above the high velocity zone and contiguous with the two deeper low velocity zones at a depth of 200-300 km above the CMB. This supports the idea that the Pacific LLSVP may be an aggregation of small upwelling plumes rather than a single large thermochemical pile.

Keywords: Waveform inversion, Western Pacific, Mantle convection, Lowermost mantle, Plume cluster

## Compressional sound velocity and density measurements of hcp-Fe under core conditions

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Sound velocity measurements of Fe and Fe-alloy at high temperature and high pressure are necessary to understand the Earth's inner core. Despite seismological observations providing density-sound velocity data of Earth's core, there are few experimental reports about sound velocity of hcp-Fe at ultrahigh pressure and temperature conditions. In order to push forward with research, we have developed a portable laser-heating system for diamond anvil cell, which is called COMPAT (Fukui et al., 2013). We have succeeded in measuring the sound velocity of hcp-iron up to 160 GPa and 3000 K by inelastic X-ray scattering measurements combining with a laser-heated diamond anvil cell. The obtained pressure and temperature dependence of the sound velocity suggest that compressional sound velocity of hcp-Fe at inner core boundary (330 GPa and 5500 K) is higher than that of Earth's inner core. Thus, we can conclude that the light elements or combination of the light elements and nickel in the inner core decreases both density and compressional sound velocity of hcp-Fe simultaneously under the inner core conditions.

### Reference

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Keywords: Earth's core, sound velocity, density, high pressure and high temperature, inelastic X-ray scattering, laser-heated diamond anvil cell

## The P-V-T equation of state of liquid pure Fe and Fe-light elements alloys by ab initio molecular dynamics simulations

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The equation of state (EoS) of pure Fe and Fe-light elements alloy liquids were calculated by means of ab initio molecular dynamics simulations at the outer core  $P$ - $T$  conditions. In the outer core, many light elements, such as carbon, nitrogen, oxygen, hydrogen, sulfur, and silicon, have been proposed as possible constituents. The concentrations of these elements have been strongly debated for years. In this study, internally consistent thermodynamic and elastic properties of pure Fe and Fe-light elements alloys, in particular density, adiabatic bulk modulus, and P-wave velocity were analyzed in order to clarify the effect of light elements incorporation on seismically observable data. Then the results were compared with the seismological data of the Earth's outer core to confine the plausible compositions of the outer core. The new EoS model of liquid iron alloys as a function of pressure, temperature and fraction of light elements may serve as fundamental data for the composition model of the Earth's core.

## Simultaneous measurement of liquid Fe-C density and sound velocity at high pressure

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The cores of terrestrial planets, such as Mercury, Mars and Moon are considered to contain some light elements. The effect of light elements on density and bulk modulus of liquid iron is necessary for estimating of these core compositions. Sound velocity of liquid iron alloys is also important for identifying light elements in the core by comparison with observed seismic data.

In this study, we have measured density and sound velocity of liquid Fe-C at SPring-8 beamline BL22XU. Density was measured using X-ray absorption method (Katayama et al., 1993) and sound velocity was measured using pulse-echo overlapping method (Higo et al., 2009). Experimental conditions were 1.2-2.9 GPa and 1650-1850 K. Obtained density values of this study were consistent with our previous results (Shimoyama et al., 2013). In sound velocity measurement, we could observe clear sample wave signal. Measured compressional wave velocity of liquid Fe-C was found to increase with pressure.

Keywords: Density, Sound velocity, liquid Fe-C

## Sound velocity and density measurement of liquid FeSi alloy by laser-shock compression

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The internal structure of the earth is estimated by observing seismic wave. Comparing seismic wave observations and experimental data of sound velocity of iron(Fe), the composition of the Earth's core is not pure Fe. Several light elements (hydrogen, carbon, oxygen, silicon, sulphur, etc.) have been considered as the candidate of the composition of the Earth's core, but its composition is still unclear. In order to constrain the core composition, it is important to measure the sound velocity of iron alloys because it can be directly compared with the seismic wave. Silicon (Si) has been proposed as a major light element in the inner core [Mao et al., 2012]. So we measured the sound velocity of laser-shocked FeSi alloy in order to investigate the effect of Si for sound velocity of liquid Fe in the outer core condition.

The starting sample was prepared by synthesizing from mixture of Fe (99.98% purity) and Si (99.9% purity) slugs at arc furnace. The compositions of Fe and Si are 66.5 wt.% and 33.5 wt.%, respectively. We measured sound velocities and densities of FeSi at high pressure and high temperature conditions at the large laser facility in Institute of Laser Engineering, Osaka University. The sound velocities were measured by the x-ray radiography [Shigemori et al., 2012].

We obtained the sound velocity and density of FeSi at pressures around 700 GPa. It is seen that Si has the effect of increasing the sound velocity of liquid Fe. Comparing our experimental results and PREM model [Dziewonski and Anderson, 1981], Si may be contained up to 13.1 wt.% at 135 GPa, and up to 5.5 wt.% at 330 GPa in the outer core.