Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-01 Room:303 Time:May 24 10:00-10:15

SHOCK-INDUCED PHASE TRANSFORMATION AND METALLIC IRON NANOPARTICLES IN OLIVINE-RICH MARTIAN METEORITES

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Maps of the magnetic field of Mars display strong magnetic anomalies attributed to crustal remanence. In order to interpret these anomalies, knowledge of the nature of magnetic carriers and magnetic properties of Martian rocks is necessary. In contrast with terrestrial rocks for which the major magnetic mineral is magnetite, studies of the SNC (Shergotty-Nakhla-Chassigny type) meteorites have shown that alternative phases, such as pyrrhotite, dominate the magnetic properties of most basaltic shergottites, while titanomagnetite is the magnetic carrier in nakhlites and a few basaltic shergottites. We studied ultrabasic SNC meteorites using low- and high-temperature magnetic property measurements and mineralogical characterization. It is shown that transformations attributed to shock cause strong modifications of olivine optical and mineralogical properties in chassignites and lherzolitic shergottites. We combined several electron microscopic techniques to fully characterize these mineralogical transformations. The observations point to transformation of olivine to a metastable high-pressure phase, possibly related to metastable transformation of olivine that were recently evidenced by X-Ray diffraction at high pressure. In the meteorites, a reduction or dissociation process of iron in olivine takes place, likely during the shock event and transformation of olivine, causing the formation of metallic precipitates in olivine. Thus, iron may be a significant magnetic carrier in Martian crust, and a precursor phase for iron-rich oxides or hydroxides in the Martian regolith.

Keywords: Martian meteorite, Shock, Olivine, Magnetism, Iron metal

SIT06-02 Room:303 Time:May 24 10:15-10:30

Contribution of volatile rich material to Earth's accretion

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The planetary formation processes such as accretion and differentiation might have drastically modified the composition of Earth from the building blocks from the orginal so-called chondritic Earth model, especially on the elemental and isotopic compositions of the volatile elements. Recently, heterogeneous accretion model that describes that growth and evolution of Earth in two different stages from volatile-depleted and volatile-rich material was revised based on isotope geochemical studies (e.g. Nudds et al., 2010). However, the exact percentage and the time sequence of this volatile-rich material accretion need to be constrained. For example, models with ~2% carbonaceous chondrite (CI-CM) material added to a dry proto-Earth will result in estimation of carbon content of Earth to be over 500ppm, which could not be explained by the current silicate mantle composition of Earth. In addition, the modeling result needs to be consistent with the siderophile elements concentration in Earth mantle and the oxidation state of Earth mantle changes through the accretion process.

Therefore, we performed experimental studied on Tagish Lake chondrite (CI-CM), a new type of volatile rich carbonaceous chondrite at different pressure and temperature conditions. Our target is to explore the possible effect of the volatile component on Earth composition through the time sequence of Earth growth, the water budge of Earth at different accretion sequences, and other possible later impact.

Our melting experiment at 12GPa shows that the measured solidus temperature of Tagish Lake meteorite is much lower than CV3 meteorite because the existence of the large amount of volatile components; however, the measured liquid temperature is very close to that of CV3 meteorite, indicating the lost of volatile component through higher temperature (2000K) heating process. The experimental method we used works well to keep the volatile components (Carbon and Hydrogen) inside the meteorite sample during heating experiments with temperature lower than 2000K. Whether does the proto-core have carbon or other volatile element will rely on further experiments at higher pressure.

Keywords: Carbonaceous chondrite, Tagish Lake meteorite, Earth accretion, High pressure and high temperature, partial melting, volatile

SIT06-03 Room:303 Time:May 24 10:30-10:45

Synthesis and application of water-bearing large single crystals by slow cooling of hydrous melt at deep mantle pressure

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The presence of water in the deep mantle of the Earth is an issue of increasing interest in the field of high-pressure mineral physics. An anticipated task for advancing the relevant research is to create homogeneous single crystals of candidate deep-mantle water-bearing minerals of 1 mm or larger in sizes, which is necessary for applying them for the Time-of-Flight (TOF) single-crystal Laue diffraction method at a third-generation pulsed neutron source. In the present study, we applied a significantly slower growth rate over a maximum period up to 24 h to successfully produce these sample crystals. We grew the crystals from a homogeneous silicate melt batch with a volume as large as possible to enable continuous buffering of chemical composition of the crystals. The temperature of the cell slowly decreased during the long heating durations so that the crystals were almost kept in chemical equilibrium with the silicate melt throughout the growth process. This slow-cooling method has been successfully applied at pressures to 24 GPa and at temperatures to about 1800 deg C, respectively, for the crystal growth of deep-mantle hydrous mineral phases. Successfully synthesized crystals include dense hydrous magnesium silicate phase E, hydrous wadsleyite, hydrous ringwoodite, and bridgmanite. These product crystals were confirmed to be inclusion free and crystallographically homogeneous. Compositional homogeneities were better than 3 % among intracrystals and intercrystals within each recovered sample capsule (Okuchi et al., in press). The product single crystals are being used for neutron diffraction as well as for another state-of-the-art mineral physics research requiring high-quality sample crystals (Goncharov et al., in press)

References

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Goncharov, A. F., S. S. Lobanov, X. Tan, G. T. Hohensee, D. G. Cahill, J. F. Lin, S. M. Thomas, T. Okuchi, and N. Tomioka, Experimental study of thermal conductivity at high pressures: implications for the deep Earth's interior, Phys. Earth Planet. Inter., in press.

Keywords: hydrous minerals, single crystal growth, phase E, wadsleyite, ringwoodite, bridgmanite

SIT06-04 Room:303 Time:May 24 11:00-11:15

Silicate Magmas under Compression and Confinement

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Upon compression and surface confinement, oxide glasses and melts are expected to be subject to successive structural transitions with multiple densification and confinement mechanisms. Experimental verification of these phenomena remain a major target of glass-melt studies. Here, we provide an overview of the recent progress and insights by solid-state NMR and inelastic x-ray scattering into structures of fluid-bearing multi-component network glasses with varying pressure, composition, and confinement (Lee et al. Rev. Min. Geochem. 78, 139, 2014); Lee Sol. St. NMR. 38, 45, 2010). In contrast to an expected complexity in densification, experimental multi-nuclear NMR results for fluid-bearing multi-component glasses at high pressure demonstrate that the pressure-induced changes in melt structures show a simple trend where the effect composition and pressure can be predicted and quantified with a network flexibility (Lee, Proc. Nat. Aca. Sci. 108, 6847 (2011)]. High-resolution O-17 NMR spectra for binary lead silicate glasses near orthosilicate composition (Pb/Si = 2), as a model system for Mg_2SiO^4 melts, reveal the presence of metal-bridging oxygen (Pb-O-Pb) and thus allow direct quantification of the degree of Mg/Si disorder (Lee & Kim, J. Phys. Chem. C, 119 748, 2015). We also report the structural evolution of andesitic and basaltic melts with varying composition, highlighting the moderate deviation from the degree of Al avoidance among framework cations (Si and Al) and preferential proximity between non-network cations (Ca_{2+},Mg_{2+}) and non-bridging oxygen. Considering all the experimental Al coordination environments available in the literature, together with the current experimental studies, we provide the relationship between the fractions of highly coordinated Al and composition, particularly average cationic potential of non-network forming cations (Park & Lee, Geochim. Cosmochim. Acta, 147, 26, 2014). Finally, as experimental evidence for thickness-induced structural transitions in amorphous oxides is lacking, we report the high-resolution NMR results for the amorphous oxides under confinement where the degree of structural disorder tends to decrease with increasing degree of confinement (i.e., near surfaces) (Lee & Ahn, Sci. Rep. 4 , 4200, 2014).

Keywords: Silicate magmas and melts, High pressure, Nuclear magnetic resonance, Inelastic x-ray scattering, Earth's interior

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-05 Room:303 Time:May 24 11:15-11:30

Spin state of iron in MORB glass up to the lowermost mantle conditions

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The existence of deep magma has been suggested by the studies of physical observations or high P-T experiments subjected to the deep Earth (e.g., Lee et al., 2010; Williams and Garnero, 1996). These melts are considered to contribute to the ultra-low velocity zone on the core-mantle boundary (CMB). However, the presence of the deep magma has been controversial yet because the physical and chemical properties of silicate melts are not understood enough under high P-T conditions.

The spin state of iron in the silicate melt is one of the important factor to affect the gravitational stability of the deep magma. The iron is one of the abundant element in the Earth and its amount is critical for the density of the silicate minerals and liquids. The iron portioning into the silicate melts was reported at pressures greater than ˜76 GPa (Nomura et al., 2011), which might cause the iron-rich dense melt above the CMB region. They suggested the iron partitioning was able to be changed due to the spin crossover of iron (from high-spin to low-spin) occurring around 70 GPa. On the other hand, some recent studies reported no spin transitions in the silicate glass at the pressures corresponding to the Earth's mantle (e.g., Mao et al., 2014; Prescher et al., 2014).

The previous studies about the spin state of iron discussed using the results limited up to the relative lower pressures (˜80 GPa) or the simple component glass expected to the actual Earth's composition. Here, we report the results of the iron spin state measurements for the multicomponent silicate glass under high pressure up to about 130 GPa, corresponding to the lowermost mantle depth. The iron spin state was measured using synchrotron ^{57}Fe M*ö*ssbauer spectroscopy method, which bring the direct information about the iron spin state.

The starting material was synthesized ^{57}Fe-enriched silicate glass, which represented an average composition of mid-ocean ridge basalt. The glass was prepared by quenching molten mixture of oxides; SiO_2, MgO, Al_2O_3, TiO_2, $^{57}Fe_2O_3$ and $CaCO_3$, K_2CO_3, Na_2CO_3. High pressure experiments were performed using a diamond anvil cell. The silicate glass powder was sandwiched between two NaCl layers which worked as a pressure medium and a pressure scale. We used equations of state for NaCl B1 and B2 phases reported by Matsui (2009) and Fei et al. (2007), respectively. In case of experiments without XRD technique, the pressure was measured based on the pressure dependence of diamond T_{2g} mode presented by Akahama and Kawamura (2004). Energy domain Synchrotron ^{57}Fe M*ö*ssbauer spectroscopy was conducted at beamline BL10XU and BL11XU of SPring-8 at room temperature and pressure ranged from 1 atm to 130 GPa. Spectra were collected for 3-11 hours depending on the data qualities. The recorded spectra were fitted with Lorentzian doublets using the MossA software package (Prescher et al., 2012).

The obtained M*ö*ssbauer spectra was able to be fitted better supposing two doublet components, which might be derived from high-spin (HS) Fe^{2+} and HS Fe^{3+}. Quadrupole splitting (QS) values of two doublets components were apt to increase from ambient condition to high pressure up to 130 GPa and were suited for the values of the previous studies. On the other hand, the change of the isomer shift (IS) had less pressure dependence.The ratio of ferrous iron to the total iron spiecies, $Fe^{2+}/\sum Fe$ showed an increase tendency up to about 60 GPa. That tendency turned to decreasing at higher pressures up to 95 GPa, and then the ratio seemed to be constant over 100 GPa. The drop of $Fe^{2+}/\sum Fe$ resembled the case of NaFe-silicate glass reported by Prescher et al. (2014) although the onset of decreasing in present study pointed at higher pressure than Prescher et al. (2014).

SIT06-06 Room:303 Time:May 24 11:30-11:45

Recent progress for stability and water solubility of hydrous and nominally anhydrous minerals in the mantle

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Recently hydrous ringwoodite was found in natural diamond inclusion, which water content was ~1.4-1.5 wt%. This shows that the mantle transition zone is really hydrous condition, at least in some regions. In addition, new dense hydrous magnesium silicate, phase H was newly found by first-principle calculation and experimental studies. Thus the study on the water in the mantle becomes a hot topic again after the finding of hydrous wadsleyite and hydrous ringwoodite.

Our group has been conducting the study for the stability and water solubility of hydrous and nominally anhydrous minerals, and the recent target is the effect of Al. In this process, we found the new Al-bearing hydrous phase in the upper mantle condition. In addition, we found that Al-bearing bridgmanite (Mg-silicate perovskite) can contain significant amount of water. So we are doing those projects to clarify the maximum water solubility in P-T conditions, structure by single crystal X-ray and power neutron diffractions, equation of state and elastic wave velocity. In this talk, we will introduce the recent progress of the water in the mantle based on our projects.

SIT06-07 Room:303 Time:May 24 11:45-12:15

Seeking constraints on lower mantle composition through nuclear resonance combined with computations

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How did the Earth form and how did it differentiate to form the core, mantle, and crust? Part of the answer to these questions resides in the composition of the present day lower mantle, where active discussions regarding how closely it approximates a chondritic composition are still ongoing. Comparison of laboratory measurements of elastic wave velocities of mantle minerals with seismic data constitutes one of the foundations upon which knowledge of the Earth's interior is based, yet it requires a precise knowledge of elastic wave velocities of the dominant lower mantle, bridgmanite, which have up until now been elusive. In situ measurements are important, because some transitions (for example, spin transitions) are not quenchable, and may influence the elastic properties of iron-containing minerals. Nuclear inelastic scattering offers the attractive possibility to determine elastic wave velocities of iron-containing minerals in the laser-heated diamond anvil cell through direct measurement of the partial density of states, although short range ordering and other effects can influence the results. We will present our measurements of elastic wave velocities in bridgmanite as a function of pressure, temperature and composition, and through comparison with ab initio calculations of the partial density of states, discuss the prospects for extracting knowledge regarding the composition and mineralogy of the present day lower mantle.

Keywords: nuclear resonance, elastic wave velocites, partial density of states, ab initio computations, bridgmanite, perovskite

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-08 Room:303 Time:May 24 12:15-12:30

Recent Advances in Understanding Elasticity of the Mantle and Core

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Elasticity of the candidate materials at the relevant P-T conditions of the Earth's mantle and core provides critical information in understanding seismic profiles and anisotropies, in building reliable compositional and mineralogical models, and in deciphering geodynamic processes and thermal history of the Earth's interior. Here I will discuss recent advances and research results in using laser and X-ray spectroscopic techniques to investigate the elasticity of candidate mantle and core materials in a high-pressure diamond anvil cell. The use of combined Brillouin and Impulsive Stimulated Scattering (ISS) results permits direct measurements of both Vp and Vs and derivation of full elastic constants of single-crystal ferropericlase and silicate perovskite up to megabar pressures. These results show that Vp of ferropericlase displays significant softening across the spin transition, while Vs is only slightly affected. The derived single-crystal C_{ij} of Bridgmanite at lower mantle pressures display relatively small elastic Vp and Vs anisotropies as compared to the ferropericlase counterpart. Furthermore, research results on the elasticity of single-crystal, polycrystalline, and textured iron alloys at high P-T conditions show that bcc-Fe and Fe-Si alloy crystals display extremely high Vp and Vs anisotropy while hcp-Fe exhibits only a few percent Vp anisotropy. Based on the expansion of the Christoffel equation, a new method to derive full elastic constants (C_{ij}) of single crystals using Vs or Vp alone will also be presented. Using thermoelastic modelling, I will discuss the elastic constants, sound velocities, elastic anisotropies, and seismic parameters of ferropericlase, Bridgmanite, and iron alloys at relevant conditions of the Earth's interior. These recent elasticity results are compared to seismic models to advance our understanding on seismic structures, mineralogical models, and geodynamic processes of the deep Earth's interior.

Keywords: Elasticity, Ferropericlase, Bridgmanite, Diamond Anvil Cell, High Pressure, Lower Mantle

SIT06-09 Room:303 Time:May 24 12:30-12:45

Compression of hcp Fe-Si-H alloy to 130 GPa

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The light elements in the Earth's core have not been identified yet, but hydrogen is now collecting more attention because recent planet formation theory suggests that large amount of water (e.g. 10 to 100 times seawater) should have been brought to the Earth during the late stage of its formation. Hydrogen is a strong siderophile element and thus it is possibly present in the core. The effect of hydrogen on the property of iron alloy is little known yet. Moreover, the presence of $\sim$ 6 wt.% silicon has been also strongly supported by geochemical and cosmochemical arguments. Here we report hydrogenation of $Fe_{0.88}Si_{0.12}$ (6.5 wt. % Si) alloy and the compression behavior of $Fe_{0.88}Si_{0.12}H_{0.8}$ alloy to 130 GPa at room temperature. $Fe_{0.88}Si_{0.12}$ foil was loaded into a diamond anvil cell (DAC), and then liquid hydrogen was introduced at temperatures below 20 K. The results demonstrate that the octahedral sites of Fe-Si-H alloys are not fully occupied by hydrogen unlike the case of FeH and as a consequence $Fe_{0.88}Si_{0.12}H_{0.8}$ is formed under hydrogen-saturated condition. The compressibility of hcp $Fe_{0.88}Si_{0.12}H_{0.8}$ is similar to that of pure iron. Assuming that liquid and solid alloys have identical density and ideal solution of hydorogen and silicon in the hcp phase, we found that the observed density profile in the outer core may be reconciled with $Fe_{0.88}Si_{0.12}H_{0.4}$. It means that the amount of hydrogen corresponding to about 90 times seawater could be in the Earth's core. This study suggests that Fe-Si-H system is a plausible chemical composition of the core.

Keywords: Light elements, Core formation, Hydorogen, Silicon, High pressure, Diamond anvil cell (DAC)

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-10 Room:303 Time:May 24 14:15-14:45

The Revolutionary Multigrain Crystallography Method for High-Pressure X-ray Diffraction

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For a century, x-ray crystallography has been conducted with one of the two extreme sample conditions: either a single crystal which produces a single set of diffraction spots directly corresponding to the geometric orientation of the crystal, or a powder sample which comprises a huge number of crystals so numerous that the diffraction spots overlap and merge into smooth rings while the geometric relation is completely lost and only the d-spacings information of diffraction planes is observed. High-pressure DAC is not optimized for either condition. Powder x-ray diffraction has the intrinsic limitations when the sample consists of multiple different phases with low symmetry. Diffraction rings cover most of the detector area, and only a couple of low angle diffraction rings are unique to a phase; most other rings overlap with one another and cannot be used for unique identification or accurate determination of crystallographic parameters. New structures and minor phases are often overshadowed by the diffraction of major phases and are impossible to find or identify. Advanced crystallographic software, such as Rietveld and LeBail refinement methods, may get most out of a powder pattern, but cannot overcome the intrinsic limitations. In addition, the common practice of integrating the 2D ring into a 1D peak plot throws away the valuable information of a whole dimension, such as the azimuthal angle of diffraction spot around the ring.

Single-crystal XRD contains orientation and geometrical relationship in addition to d-spacings and thus provides a definitive characterization of the unit cell and symmetry. Unless the crystal is orientated exactly relative to the incident monochromatic x-ray beam to satisfy the Bragg relation, the crystal gives no signal, and the detector remains empty. Rotating the crystal around the w-axis (perpendicular to the incident x-ray beam) can bring the crystal to Bragg condition and occasionally obtain single diffraction spots at a given angle and scanning step. In spite of the advantages, single crystal cannot be sustained through phase transitions and often breaks down into multiple crystals and generate spotty XRD patterns.

Spottiness, that is generally regarded as a flaw in powder XRD, can be turned into great advantages if we can separate individual crystallites and handle them as individual single crystals. The high-brilliance x-ray beam available at synchrotron facilities has made it possible to collect diffraction spots in a powder sample comprised of up to hundreds of submicron crystallites. The newly developed Multigrain Crystallography (MGC) package, which is a suite of programs used for processing and indexing diffraction spots, has been developed to separate and identify the crystallographic orientation of each individual crystallite in the aggregate of hundreds of crystallites. Once separated, the data set for each crystallite can be handled with the standard single-crystal refinement program identical to a stand-alone single crystal, resulting in excellent statistics in refinement and full coverage of the reciprocal space. The MGC method is very powerful in unequivocal determination of symmetry and unit cells, testing different indexing models, picking out minor phases, and resolving strain of individual crystallites, and will very likely replace the powder and single-crystal x-ray diffraction methods as the dominant crystallographic tool for future high pressure-temperature studies in DAC.

Keywords: High pressure X-ray diffraction, Crystallography

SIT06-11 Room:303 Time:May 24 14:45-15:00

Effective metal-silicate equilibrium temperature during core formation

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It has been long known that the formation of the core transforms gravitational energy into heat and is able to heat up the whole Earth by about 2000 K. However, the distribution of this energy within the Earth is still debated and depends on the core formation process considered. Iron rain in the surface magma ocean is supposed to be the first mechanism of separation for large planets, iron then coalesces to form a pond at the base of the magma ocean. In this process, equilibrium between metal and silicate is achieved within several seconds [Ichikawa et al., 2010].

Experimental studies of metal-silicate partition coefficient show that pressure-temperature conditions for metal-silicate equilibrium are far beyond the liquidus or solidus temperature for several hundred kelvin [e.g. Wade and Wood, 2005]. However, because equilibration was considered to occur in at the surface of metal pond at the silicate solidus, such high temperature equilibration was rejected as implausible. Instead, lower temperature equilibration with variable oxygen fugacity was proposed as an alternative, although the plausibility of the physical mechanisms invoked in this scenario is also questionable.

In this study, we model iron rain and heating of the magma by viscous dissipation to calculate the effective pressure-temperature conditions for partitioning in this scenario based on parameterizations derived from direct numerical simulation results of a 10cm-scale emulsion of liquid iron in liquid silicates. We have found effective temperature is much higher than melting temperature of silicate due to the release of gravitational potential energy.

Keywords: magma ocean, metal-silicate equilibrium, iron rain, numerical simulation

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-12 Room:303 Time:May 24 15:00-15:15

On the core-mantle thermo-chemical evolution with the basal magma ocean in the early Earth

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On the recent progress of melt phase relationship such as the density structure of silicate melt in the deep mantle [e.g. Stixrude et al., 2009], the density of silicate melt would be much denser than the silicate solid near the core-mantle boundary (CMB), which has been already proposed from high pressure experiments [e.g. Ohtani and Maeda, 2001]. As a result, the basal magma ocean hypothesis for thermo-chemical structure in the early Earth has been proposed in several years ago, which is based on the concept for the density cross-over between silicate melt and solid in the deep mantle [Labrosse et al., 2007]. In this study, we attempt to include melt-phase relationship in the mantle minerals into a coupled core-evolution model based on numerical mantle convection simulations, which can generate the basal magma ocean in the early Earth. The preliminary outcome from this modeling is that the survival time-scale of the basal magma ocean in the mantle convection system is around 2.0 Gyrs as well as low CMB heat flow (~5 to 10 TW) at the present time compared to the expected from theoretical core evolution model including the basal magma ocean. On the survival time of basal magma ocean obtained here, the origin of ultra-low-velocity-zone is difficult to generate the partial melting survived over the geologic time-scale, which seems to be explained as the compositional difference (effects of iron) suggested from recent seismological data analysis [e.g. Brown et al. 2015]. On the heat flow across the CMB, it is similar results to cases without assuming the effect of basal magma ocean suggested that the early Earth hypothesis would be still difficult to explain the various diagnostics of Earth's core-mantle evolution over the geologic time-scale.

Keywords: Thermal evolution of Earth's core, Basal magma ocean, Melt phase relationship, Mantle dynamics, Early Earth

SIT06-13 Room:303 Time:May 24 15:15-15:30

Silicate melts of the Earth's mantle

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We explore the state of various silicate melts, with different realistic compositions, characteristic for various moments of the crystallization of the magma ocean. Using a starting basis of silica tetrahedra we vary the amount and the quality of the cations, including trace elements.

For this, we employ first-principles molecular dynamics simulations. We perform spin-polarized calculations in the planar augmented wavefunction formalism of the density-functional theory, using the VASP package.

We monitor the dependence with pressure and temperature of various physical parameters, like density, coordination number, magnetic spin, viscosity, etc. We show that the coordination number in the silicate groups increases from 4 to 5 to 6 as we go from ambient pressure to megabar. We estimate the thermal dilatation; from the equations of state we compute the velocities of the compressional seismic waves. We use these results to show that melts can still exist at the base of the Earth's present-day lower mantle as iron-rich pockets. These melts can explain particular features, characterized by low seismic velocities, such as the ultra-low velocity zones. Using the more complex chemistries we provide the first insights into the behavior of the magma ocean during cooling and crystallization.

Keywords: mantle, silicate, melt, spin transition, equation of state, magma ocean

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-14 Room:303 Time:May 24 15:30-16:00

Single-crystal Brillouin Spectroscopy with Laser Heating and Variable q: Design and Results on Olivine

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We have developed a novel Brillouin spectroscopy system integrated with CO2 laser heating and Raman spectroscopic capabilities. High-pressure laser heating experiments on liquid water compressed in a diamond-anvil cell up to 2500 +/- 150 K demonstrate the flexibility and performance of the system. Temperature is determined from the grey-body thermal radiation of the heated samples. New single-crystal laser heating Brillouin measurements were made on San Carlos Olivine in the (111) plane at pressures up to ~13 GPa, and T=1300K. We obtain quantitative values for the thermal pressure in the diamond cell. Using KCl and KBr and pressure-transmitting media, we show that pressure gradients in the sample chamber are small at high P-T conditions based on observations of the olivine-wadsleyite transition. This system is additionally designed for continuously varying scattering angles from near forward scattering (0o scattering angle) up to near back scattering (~141o). Our results on the sound velocities of olivine at high pressure-temperature conditions have implications for the nature of the 410 km discontinuity and the olivine content of the transition zone.

Keywords: Elastic properties, Brillouin scattering, Equations of state, Olivine

SIT06-15 Room:303 Time:May 24 16:15-16:30

Estimation of dislocation mobility in different slip systems in olivine as a function of pressure and temperature

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It is considered that the seismic anisotropy in the upper mantle will be caused by crystallographic preferred orientation of olivine. The seismic anisotropy rapidly decreases below 200 km depth, which is attributed to a transition from A-type to B-type fabric with pressure indicated by deformation experiments. However, stress and strain-rate conditions in deformation experiments are by orders of magnitude higher than in the upper mantle, which may mislead our understandings.

A- and B-type fabrics are produced by the dominant slip systems of (010)[100] and (010)[001], respectively. Hence, the fabric transition implies that the dislocation mobility in (010)[100] will decrease with increasing depth more than in (010)[001]. In order to examine this hypothesis, we determined the dislocation mobility of (010)[100] edge (a-dislocation) and (010)[001] screw (c-dislocation) dislocations at pressures of 0 to 12 GPa and temperatures of 1470 to 1770 K by means of the dislocation recovery technique, in which the dislocation mobility is determined under quasi-hydrostatic conditions. The a- and c-dislocations were produced in (010)[100] and (010)[001] simple shear geometries by 45-degree-edge alumina pistons at a pressure of 3 GPa and a temperature of 1600 K for one hour. TEM observations indicated that 90 % of dislocations produced in (010)[100] and (010)[001] simple shear geometries are a- and c-dislocations, respectively.

The experimental results show: (1) The mobility of a-dislocation is almost identical to or up to 0.5 orders of magnitude lower than that of c-dislocation at ambient pressure. (2) The activation energies of both dislocations are comparable, about 400 kJ/mol. (3) The activation volumes of both dislocations are also comparable, about 2.6 cm3/mol.

The comparable activation energies and volumes suggest that the transition of A-type to B-type fabric by pressure and/or temperature is unlikely. The rapid decrease in seismic anisotropy below 200 km will be due to decrease in flow rate in this depth.

Keywords: olivine, dislocation, mobility, pressure, temperature

SIT06-16 Room:303 Time:May 24 16:30-16:45

Experimental constraints on the chemical compositions of the mantle transition region and the lower mantle

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Technical developments in mineral physics using Kawai-type multianvil have been made for precise determinations of phase transitions and associated density/velocity changes in high-pressure minerals under the pressure and temperature conditions toward the deeper region of the mantle. We have been studying these properties in materials relevant to the mantle and subducted slabs, which provides tight mineral physics constraints on the chemical compositions of the deep mantle. The results indicate that the mantle transition region, as well as the upper manatle, is made of a pyrolitic composition except for its bottom region, where the existence of materials with higher sound velocities is suggested to account for one-dimensional seismological models such as PREM. As for the deeper region of the mantle, our recent sound velocity measurements on bridgmanite (Higo et al., in prep.) shows that the lower mantle should also have a pyrolitic composition, rather than the more silicon-rich composition close to pyroxene stoichiometry as concluded in a recent work based on Brillouin scattering measurements. This result is consistent with a prediction based on ab initio calculations, suggesting that the bulk mantle of the Earth is significantly depleted in Si relative to CI chondrites.

Keywords: high pressure experiment, mantle transition region, lower mantle, mineral physics, elastic velocity, pyrolite

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-17 Room:303 Time:May 24 16:45-17:15

Metallic Fe and its influence on melting in the lower mantle

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Melting in the deep Earth has important influence on the chemical evolution of Earth. Melting in the deep Earth is largely controlled by the availability of volatile (incompatible) elements that selectively go to the melt. In most of the lower mantle, melting will be difficult without volatiles. However, if a small amount of volatiles is present, melting becomes very easy and partial melting is expected in most lower mantle if volatiles are present.

Such a situation will be dramatically modified, if metallic Fe is present as first shown by Frost et al. (2004). These authors showed that metallic Fe is produced in the lower mantle assembly and that the formation of metallic Fe is not caused by the removal of oxygen but rather caused by the internal transfer of electrons due to the high stability of ferric Fe in bridgmanite. If this reaction occurred throughout the lower mantle, partial melting will be hard.

In this talk, we will present new experimental observations suggesting that the formation of metallic Fe is highly pressure dependent and it occurs only in the shallow lower mantle. The experimental results are the heterogeneous distribution of metallic Fe in a sample assembly in RDA where substantial pressure gradient is present. Metallic Fe is observed only in the low-pressure regions (24-26 GPa), whereas metallic Fe is not detected in the high-pressure regions (>27 GPa). We developed models to explain these observations that also explain varying results of previous studied at different pressures.

We conclude that a substantial amount (~1 % or larger) of metallic Fe is present only in the limited depth region in the lower mantle (660 to ~730 km). A possible implication of this observation to explain seismological observations by Schmandt et al, (2014) will be discussed.

Keywords: melting, lower mantle, volatile elements, metallic Fe

SIT06-18 Room:303 Time:May 24 17:15-17:30

Thermal equations of state of $MgSiO_3$ post-bridgmanite phase

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$MgSiO_3$ post-bridgmanite phase exists at the lowermost mantle of the Earth. Thus many studies on the equation of state of the phase were done at the lowermost mantle P-T conditions (Caracas and Cohen, 2008; Guignot et al., 2007; Oganov and Ono, 2004; Ono et al., 2006; Tsuchiya et al., 2004; Mosenfelder et al., 2009). On the other hand, super-Earths which have a few times of the Earth's mass have been found in the extra solar system one after another. $MgSiO_3$ post-bridgmanite is an abundant silicate phase in such huge terrestrial planet's mantle (Tsuchiya and Tsuchiya, 2011). Although the pressure condition of super-Earth's mantle reaches several hundred GPa, previously reported EoSs of post-bridgmanite by the laser heated diamond anvil cell (LHDAC) experiment were limited up to around 150 GPa. Moreover, the post-bridgmanite is expected to exist in Uranus's and Neptune's rocky cores and also early Earth's proto-core. The direct determination of the compression behavior of post-bridgmanite at multi-megabar pressure is, therefore, important to understand the super-Earth's interior and so on.

Here we report PPv EoSs up to 258 GPa and 2140 K based on the LHDAC experiment and up to 1 TPa and 6000 K by ab initio calculation based on the density-functional theory in the same manner as Tsuchiya et al. (2004). The experimental EoS agrees excellently with the calculated ab initio volume data within 1% up to 400 GPa and 6000 K. The volume differences between the present result and the EoS based on shock experiment data (Mosenfelder et al. 2009) was also 1% at 400 GPa and 300 K. The present EoSs show internal consistency among LHDAC, shock and ab initio data up to 400 GPa within 1% in volume. Our new EoSs are applicable to not only the Earth's core-mantle boundary region but also the super-Earth's mantle and early Earth's proto core.

Keywords: post-bridgmanite, equation of state, LHDAC, Ab initio calculation

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-19 Room:303 Time:May 24 17:30-18:00

Core Formation Process and Composition of the Core

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Geochemical and cosmochemical arguments imply that major candidates of the light elements in the core are Si, O, S, and H with small amount of hydrogen. In the early stage of the planetary formation, the core formation process started by percolation of the metallic liquid though silicate matrix (1). The planetesimals which built the Earth could have a composition similar to enstatite chondrite, which contains some amount of sulfur as sulfide such as troilite, CaS, and metallic iron under reducing conditions. Therefore, the in the early stage of the accretion of the planetesimals, the Fe-FeS eutectic liquid could be formed and separated to the core by the percolation process. The major light elements of the core at this stage will be sulfur.

The internal pressure and temperature increased with the growth of the earth, and metallic iron depleted in sulfur was molten. The molten metallic iron can dissolve both Si and O as was experimentally shown by several authors (2). The core forming metallic liquid sunk into the bottom of the magma ocean and was in equilibrium with the magma ocean at high pressure around 40-60 GPa (3). The core separation occurred by the Rayleigh-Taylor instability. The core contains S, Si, and O by this process. If small amount of water was trapped in the magma ocean, most of H can be absorbed by the metallic core by strong partitioning of H into the metallic iron (4), and the magma ocean would have become dry.

The partitioning experiments between solid and liquid iron alloys indicate that S is strongly partitioned into the liquid outer core, whereas O is weakly into the liquid outer core, and Si into the solid inner core. H contents in the outer and inner cores are nearly the same due to similar H contents in solid and liquid iron (4). Based on the partitioning behavior between the outer and inner cores, the equation of state, and sound velocity of iron-light element alloys, the plausible distributions of the light elements in the outer and inner cores are examined.

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Keywords: formation process, planetesimal, magma ocean, light element, outer core, inner core

SIT06-20 Room:303 Time:May 25 09:00-09:15

High-pressure polymorphs of silica in shocked meteorites and their implications

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A high-pressure polymorph of silica is one of most unambiguous evidences for an impact event. Natural coesite and stishovite were discovered from impact craters on the Earth for the first time. Some meteorites are heavily shocked. Recent our studies reveal that high-pressure polymorphs of silica occur in many kinds of meteorites. Stishovite and coesite were identified from a lunar meteorite, Asuka 881757 for the first time (Ohtani et al., 2011). Subsequently, α-PbO_2 type silica, seifertite along coesite and stishovite were found from a lunar meteorite, NWA 4734 (Miyahara et al., 2013). In addition to lunar meteorites, we also identified stishovite from a lunar return sample, Apollo 15299 breccia (Kaneko et al., 2014). Considering radio-isotope chronology, the high-pressure polymorphs of silica are closely related with the late heavy bombardment and subsequent meteoroid impacts on the Moon. Miyahara et al. (2014) identified coesite and stishovite from eucrite which was expected to originate from 4 Vesta, which raised an objection about howardite-eucrite-diogenite delivery model to the Earth. Coesite and stishovite are also found from enstatite and carbonaceous chondrites (Weisberg et al. 2010; Kimura et al., 2014) although their parent-bodies are expected to be less shocked. Now the existences of coesite and stishovite in shocked meteorites appear to be ubiquitous. Therefore, high-pressure polymorphs of silica, which were overlooked, will become a new clue for clarifying a dynamic event in the solar system. On the other hand, the pervasive existence of coesite in shocked meteorites is enigmatic. The phase transition from quartz to coesite is not easily achieved in a transient high-pressure condition due to a high kinetic barrier (e.g., Mosenfelder and Bohlen, 1997). Coesite occurs in a silica grain entrained in a shock-melt vein or melt-pocket. Most coesite are un-oriented fine-grained assemblages accompanying silica glass. Coesite in shocked meteorites may crystallize from silica-glass or melt subsequent to amorphization or melting. Coesite probably has a high nucleation rate in silica-glass or melt.

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Keywords: silica, high-pressure polymorph, meteorite

SIT06-21 Room:303 Time:May 25 09:15-09:30

Liquidus phase relations in MgO-FeO-SiO2 system at high pressure: Implications for the solidification of magma ocean

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Seismological observations show the presence of large anomalies in the lowermost mantle such as LLSVP and ULVZ, both of which should be denser than surrounding mantle and thus gravitationally stable. The origins of such anomalies are still under debate, but they could be related to a basal magma ocean (BMO) that may have formed in early history of the Earth; the LLSVP represents iron-rich solids crystallized from the evolved BMO, and the ULVZ is a residual melt left after extensive solidification of the BMO.

Here we performed high-pressure melting experiments on the MgO-FeO-SiO_2 ternary system in a laser-heated diamond-anvil cell (DAC). Chemical and textural characterization of recovered samples were made using dual beam scanning microprobe (FIB + FE-SEM) (Versa 3D) and field-emission-type electron probe microanalyzer (FE-EPMA). The cross section of the sample showed a round portion with non-stoichiometric composition at the center (the hottest part), which represents quenched partial melt. And, such quenched melt was surrounded by a layer of solid phase(s) of (Mg,Fe)SiO_3 bridgmanite, (Mg,Fe)O ferropericlase, and SiO2 stishovite. Together with previous theoretical calculations of eutectic melt compositions in MgO-SiO_2 binary system and experimental results on FeO-SiO_2 and $(Mg,Fe)_2SiO_4$ systems, the liquidus phase relations in the MgO-FeO-SiO_2 ternary system were determined at 36 GPa. We also estimated those at 135 GPa considering the increase in iron content in bridgmanite with increasing pressure.

These results indicate that residual melt of the BMO should have evolved toward iron-rich and silica-poor with solidification. Fractional crystallization in the BMO leads to a very small fraction of residual melt that is strongly enriched in FeO, which is very dense in the lowermost mantle. The knowledge of chemical evolution of the BMO help understand the nature of the LLSVP and the ULVZ.

Keywords: magma ocean, mantle evolution

SIT06-22 Room:303 Time:May 25 09:30-10:00

A coordinated study on structures of liquids/glasses using synchrotron radiation in Paris-Edinburgh and the diamond cell

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Structures of geo-liquids at temperature and pressure conditions of the deep interior of the Earth fundamentally control the physical properties of these liquids, which, in turn, profoundly influence chemical and thermal evolution of the Earth. We have developed a suite of monochromatic x-ray diffraction techniques using both a Paris-Edinburgh press (PEP) and a diamond anvil cell (DAC) at the GSECARS beamlines. With two high resolution Si (111) and (311) monochromators, a multi-channel collimator (MCC) assembly, and two Kirkpatrick-Baez focusing mirrors, we have an exciting opportunity for liquid and glass structure studies in both the PEP and the DAC. A new PEP anvil geometry has been adopted which is capable of generating pressures in excess of 15 GPa on 0.5 mm diameter samples. Cell assemblies have been developed and temperatures up to 2000 C have been maintained over hours. A simple analysis shows that with a finely collimated or tightly focused incident beam of 0.05 mm, a collimation depth of 0.5 mm can be achieved at two-theta angles above ˜10 degrees with the MCC. The PEP is mounted on the general-purpose diffractometer (GPD) in 13-ID-C, with the sample located at the center of the six-circle diffractometer, which allows scanning an area detector (e.g., MAR CCD) to cover maximum Q range up to 30 $Å^{-1}$,with x-ray energies above 60 keV. Ultrasonic acoustic velocity measurements can be conducted in-situ at high pressure and temperature to study elasticity of liquids using either the PEP or other large-volume, high-pressure devices. Applying a similar diffraction setup for the DAC technique, we can now study structural evolution of super-cooled liquids (glasses) to pressures in excess of 150 GPa both at room temperature and high temperatures. With a focused incident beam on the order of 0.03 mm, the MCC effectively reduces unwanted Compton scattering of the diamond anvils by a factor of 10, thereby allowing more accurate extraction of x-ray total scattering signals from tiny samples. Furthermore, online Brillouin spectroscopy allows acoustic velocities to be measured under the same pressure and temperature range. We will present results on structural responses and densification mechanisms of a number of silicate liquids and glasses at high pressures. Implications for melt dynamics in the Earth's interior will be discussed.

Keywords: synchrotron, high pressure, liquid structure, diffraction, early earth, mantle dynamics

SIT06-23 Room:303 Time:May 25 10:00-10:15

Acoustic wave velocity measurements of SiO_2 - Al_2O_3 glasses up to 200GPa

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Determination of the structure and physical properties of silicate melt under high pressure and high temperature is an important key to understand the stratified structure of the Earth through the global magma ocean in early Earth, and the gravitational stability of melts in Earth′s deep mantle. Natural silicate melts mainly consist of SiO_2 with various chemical components. Al_2O_3 is one of the most abundant components in natural silicate melts after SiO_2 (e.g., Mysen, 2005). Thus, it is essential to understand the effect of Al_2O_3 on the density and the structure of silicate melts under the high pressure and high temperature condition corresponding to the Earth′s mantle. However, the density and the structure of silicate melts under the whole mantle condition are poorly understood, and it is unclear whether an aluminous silicate melt is buoyant or not in a certain mantle condition.

In this study, in-situ high-pressure acoustic wave velocity measurements of SiO_2-Al_2O_3 glass were performed up to around 200 GPa using Brillouin scattering spectroscopic techniques to understand the effect of Al_2O_3 on pressure-induced structural changes in silicate glasses, as the analogue of silicate melts, under the whole mantle pressure conditions. We used both SiO_2 + 3.6 mol% Al_2O_3 glass (SA1) and SiO_2 + 20.0 mol% Al_2O_3 glass (SA2) as a starting material, synthesized using container-less liquid phase processing at the SPring-8 BL04B2.

The results below 30-40 GPa showed that the acoustic wave velocity of SA1 and SA2 increases with increasing Al_2O_3 content at a certain pressure, showing that the difference of bulk modulus (K) and shear modulus (μ) occurs depends on Al_2O_3 content in SiO_2-Al_2O_3 glasses. It is suggested that K, μ and of SiO_2 - Al_2O_3 glasses become large with progressing depolymerization in this pressure range.

At the pressures from 30-40 GPa to 100 GPa, the velocity increase with pressure is more gradual. Above 100 GPa, the sharp increase in the velocity gradient were observed in both SA1 and SA2. The pressure at which the sharp increase in the velocity gradient occurs are 130 $\pm$ 5 GPa in SA1, and 116 $\pm$ 9 GPa in SA2, and these values are smaller than those of SiO_2 glass and $MgSiO_3$ glass (Murakami and Bass, 2010; Murakami and Bass, 2011). The pressure condition at which the change of the velocity gradient occurs in SA1 are 10 GPa lower than that in SiO_2 glass and 3 GPa lower than that in $MgSiO_3$ glass. Moreover, such pressure condition in SA2 are 24 GPa lower than that in SiO_2 glass and 17 GPa lower than that in $MgSiO_3$ glass. This result may suggest that Si ions have a coordination number greater than 6 in both SA1 and SA2 around above mentioned pressures, and Al_2O_3 could lower the pressure condition for the formation of the Si-O coordination numbers higher than 6. The results suggest that an aluminous silicate melt is likely to become dense at much shallower depth than CMB.

Keywords: Structure of silicate glasses and melts, Brillouin scattering, Acoustic wave velocity measurement

SIT06-24 Room:303 Time:May 25 10:15-10:30

High-pressure radiative conductivity of dense silicate glasses with implications for dark magmas

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The current structure of Earth's interior is believed to have developed through dynamic differentiation from a global magma ocean in the early Earth. Elucidation of the heat-transport properties of silicate melts in the deep Earth is fundamental to understanding the evolution and structure of Earth's interior. The possible presence of dense, gravitationally stable, silicate melts at the bottom of the current mantle, as a remnant of a deep magma ocean, has been proposed to explain observations of anomalously low seismic velocities above the core-mantle boundary. Thus, heat flux through the core-mantle boundary (CMB) region would strongly depend on the thermal conductivity, both lattice-vibrational and radiative , of such dense silicate melts, as well as that of constituent minerals of the lower mantle. However, the thermal properties of such silicate melts under relevant high-pressure conditions are poorly understood, while there have been several experimental studies on the thermal conductivity of lower mantle minerals such as magnesium-rich silicate perovskite (bridgmanite) and ferropericlase. Direct measurements of thermal conductivity on silicate melts under ultrahigh-pressure conditions remain a great challenge and are currently beyond experimental capabilities. Alternatively, silicate glasses have been studied as analogues for quenched silicate melts, to simulate high-pressure melt behavior. Previous experimental works on silicate glasses have, however, been still limited to lower pressure condition, which is far below the pressure condition of the bottom of the mantle.

Here we report in-situ high-pressure optical absorption and synchrotron Mossbauer spectroscopic measurements of iron-enriched dense silicate glasses, as analogues for dense magmas, up to pressures of 85 GPa. Our results reveal a significant increase in absorption coefficients, by almost one order of magnitude with increasing pressure to about 50 GPa, most likely due to gradual changes in electronic structure. This indicates that the radiative thermal conductivity of dense silicate melts may decrease with pressure and so may be significantly smaller than previously expected under the CMB conditions. Such dark magmas heterogeneously distributed in the lower mantle would result in significant lateral heterogeneity of heat flux through the CMB.

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-25 Room:303 Time:May 25 10:30-10:45

Single-crystal elastic property of bridgmanite and seismic anomalies in the lower mantle

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Single crystal elasticity of bridgmanite is essential information to understand the seismic velocity structure of the lower mantle from the viewpoint of chemical and thermal structures. We have performed inelastic x-ray scattering measurement at BL35XU of SPring-8 on 100-micron size (Mg,Fe,Al)(Si,Al)O_3 single crystals synthesized by thermal gradient method. Analysis of the obtained spectra gives single crystal elastic stiffness constants. The cation substitution is seen to cause the anti-correlation between the bulk sound and shear wave velocities as well as to enhance the elastic anisotropy of bridgmanite, and consequently allows us to make a quantitative model that is consistent with seismological observations.

Keywords: bridgmanite, inelastic x-ray scattering, single crystal elasticity, cation substitution, lower mantle, seismic anomaly

Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

SIT06-26 Room:303 Time:May 25 11:00-11:30

Melting and core formation during accretion of the Earth

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The most significant differentiation event in the history of the Earth resulted in the formation of the Earth's iron-rich core and silicate mantle. Core formation involved the segregation of metal from silicate for which high temperatures were required. At least the metal, and probably also the silicate, had to be in a molten state for segregation to occur efficiently. Although the decay of short-lived isotopes provided sufficient heat for the core-mantle differentiation of early-formed planetary bodies, this heat source was only effective during the initial 2-3 My of Solar System history. The heat required for core-mantle differentiation of the Earth was derived primarily from high-energy collisions with other planetary bodies that culminated in the Moon-forming giant impact.

In order to study the compositional evolution of the growing planets, we have combined N-body accretion simulations with a model of multistage core formation (Rubie et al., 2015, Icarus 248, 89-108). Impacts of embryos and planetesimals with growing proto-planets are considered to result in large-scale melting, magma ocean formation and an episode of core formation. Metal-silicate equilibration at high pressure and temperature results in equilibrated metal and silicate compositions that are determined by mass balance combined with element partitioning data. The evolving compositions of the mantles and cores of the terrestrial planets can thus be modelled simultaneously. Model parameters are constrained by fitting the final composition of the mantles of Earth-like planets to the composition of the Earth's primitive mantle. However, current results are based on the simplifying assumption that metal-silicate equilibration pressures are always a constant fraction (typically around 0.7) of the proto-planet's core-mantle boundary pressure.

In order to further develop the model of Rubie et al. (2015), we are now calculating the depth of melting for each impact in the N-body simulations, which enables the P-T conditions of metal-silicate equilibration to be specified. Full three-dimensional models of planetary collisions are computationally too time-consuming for the large number (hundreds to thousands) of impacts in the N-body accretion simulations. Two-dimensional models cannot be used for non-vertical impacts due to their assumed symmetry in the third dimension. Therefore, a parameterised model is used which describes the amount and depth of melting based on the energy needed to melt a dunite mantle together with the energy provided by the impact. The available energy depends on the impact angle and velocity as well as on the impactor mass and the material properties of the impactor and the target.

A deep melt pool, formed by a collision between bodies of similar size, will spread over the planet's surface to form a global magma ocean as the result of isostatic readjustment. Subsequent planetesimal impacts may occur while this magma ocean is still present, in which case metal-silicate equilibration will take place near its base. With a simple cooling model, an estimate can be made of the depth of the magma ocean as a function of time. Using this method, equilibration temperatures and pressures are calculated for each impact. This approach is being used to constrain the accretion history and the presence or absence of a dense insulating atmosphere during the early history of the Earth.

Keywords: magma oceans, giant impacts, differentiation, high pressure