Crystal chemistry of hydrogen and water storage in planetary interiors

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The crust and mantle of the Earth are made of oxygen minerals. Hydrogen solubility in these minerals controls the abundance of water on the surface and hence the possibility of life on terrestrial planets. Hydrogen can be incorporated in nominally hydrous minerals such as Phase B, superhydrous phase B, phase D, and phase H, or in nominally anhydrous minerals. In the upper mantle and transition zone, the nominally anhydrous minerals may be the principal host phases for H and are capable of incorporating many times the amount of water in the surface oceans.

In the nominally anhydrous minerals at the atomic scale H does not behave like any other cationic substituent. It bonds to a single oxygen with an inter-nuclear distance of less the nominal radius of the oxygen anion to form a hydroxyl anion. Although it does require charge balance, typically a cation vacancy, it does not substitute at cation sites. This has significant impact on elastic properties. The cation vacancies increase the molar volumes and decrease density as well as bulk and elastic moduli. By measurement of the effects of hydration on elastic properties of the nominally anhydrous major minerals of various regions of the mantle it possible to estimate the presence of water. The velocity structure of the Earth is consistent with significant hydration in the upper mantle and transition zone.

In nominally hydrous minerals, with a few notable exceptions, the hydroxyl does not bond to Si, or other high-charge cations, such as C, N, P, or S. In nominally anhydrous minerals, oxygen sites that can be partially protonated to form the hydroxyl can be predicted from Madelung electrostatic site energy calculations. These calculations predict significant hydration in wadsleyite and ringwoodite and limited hydration in olivine. They also predict potential limited hydration in bridgmanite.

Keywords: Water, Crystal Chemistry, Earth's interior

Role of water in subduction zone magmatism

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Arc magmas are hydrous reflecting water from the subducted oceanic plate and subsequent hydrous melting of the mantle. Both water and water-mobile elements are rich in the arc magmas which exert formation of the arc’s crust thus the Earth’s continent. Arc magmatism is a complex process occurring in such the dynamic system with the enigmatic water-bearing chemical reactions. This presentation aims to describe the processes of arc magma genesis based on chemical mass balance between the magmas and their source materials. The petrology/geochemistry-based mass balance model uses elemental-isotopic compositions and explores intensive-extensive parameters which control the chemistries. The determined parameters are then used to constrain the genetic conditions of the arc magmas and the dynamics of both the liquids and solids. The examinations focus on the contrasting NE and SW Japan arcs where the globally coldest and the hottest endmember subductions are taking place.

Keywords: Subduction zone, Water, Magma

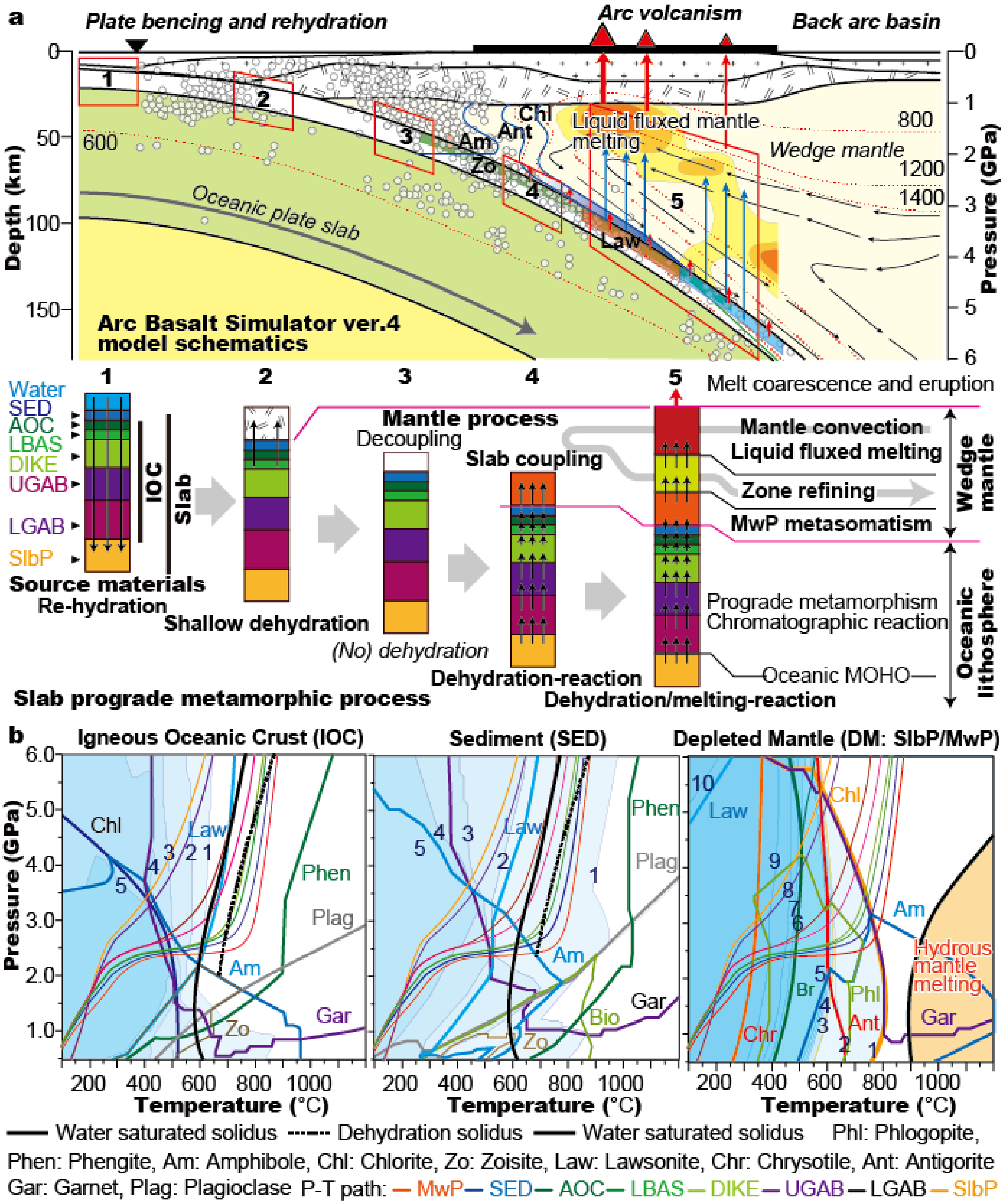

Fig. 4.4.1 Schematic cross section of a subduction zone and the Arc Basalt Simulator ver.4 model description (panel a). Phase relations and maximum bound water in igneous oceanic crust, sediment, and depleted peridotite (panel b), modified from Kimura et al. (2012). Acronyms of the slab layers are MwP: mantle wedge peridotite, SED: sediment, AOC: altered oceanic crust, LBAS: lower basalt, DIKE: dike, UGAB: upper gabbro, LGAB: lower gabbro, and SlbP: slab peridotite.

Mantle melting and volatiles: Redox-controlled solution behavior in silicate-COH magmatic systems

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The behavior of hydrogen-bearing fluids and magmatic liquids is at the core of understanding formation and evolution of the Earth, its oceans, and atmosphere. To advance this knowledge, infrared and Raman spectroscopy has been employed for melt structural characterization and for determination of hydrogen and carbon isotope partitioning within and between melts and fluids in alkali aluminosilicate–C-O-H systems contained in externally-heated diamond anvil cells. The measurements were carried out in-situ under equilibrium conditions while the samples were at the temperatures, pressures, and redox conditions corresponding to those of the Earth’s upper mantle and deep crust.

Hydrogen as H_2O is the major component of the silicate Earth. Its solubility in magma can reach >30 wt% under crustal and upper mantle conditions. The CH_4 and H_2 solubility is in the 0.1-1 wt% range, and CO_2-solubility typically 1-5 wt%. These variations reflect bulk chemical and, therefore, structural control of solubility. Water dissolved in magmatic liquids to form predominantly Si-OH and Al-OH bonding together with molecular H_2O. The OH/H_2O ratio is positively correlated with SiO_2 and Al_2O_3 concentrations in melts. The carbon solution equilibria are, $2CH_4+Q^n=2CH_3+H_2O+Q^{n+1}$ and, $2CO_3+H_2O+2Q^{n+1}=HCO_3+2Q^n$, under reducing and oxidizing conditions, respectively. In the Q^n-notations, the superscript, *n*, in the Q^n-species denotes number of bridging oxygen in the silicate species (Q-species). The abundance ratios, CH_3/CH_4 and HCO_3/CO_3, increase with temperature.

The resulting structural changes result in hydrogen and carbon isotope fractionation factors between melt, fluid, and crystalline materials significantly different from 1 even at magmatic temperatures. The D/H and fractionation between aqueous fluid and magma are also temperature dependent with a small enthalpy change near -5 kJ/mol. In silicate-C-O-H systems, the enthalpy-values for $^{13}C/^{12}C$ fractionation factors are near -3.2 and 1 kJ/mol under oxidizing and reducing conditions, respectively. These differences reflect different energetics of O-D, O-H, O-^{13}C, and O-^{12}C bonding environments governed by different solution mechanisms in melts of the individual volatile components.

From experimentally-determined temperature- and pressure-dependent D/H fractionation between fluids and melts, it is suggested suggest that (C-O-H)-saturated partial melts in the upper mantle can have dD-values 100%, or more, lighter than coexisting silicate-saturated fluid. This effect is greater under oxidizing than under reducing conditions. Analogous relationships exist for $^{13}C/^{12}C$ with $\partial^{13}C$-differences between silicate melts and coexisting CO_2+H_2O (oxidizing) and $CH_4+H_2O+H_2$ (reducing) fluid and at magmatic temperatures in the Earth’s upper mantle increases with temperature from about 40 to > 100‰ and 80 –120 ‰under oxidizing and reducing conditions, respectively. The use of hydrogen and carbon isotopes of mantle-derived magma to derive isotopic composition of upper mantle source regions, therefore, is discouraged as these are affected by temperature, bulk composition, and redox conditions during melting, crystallization, and degassing events.

Keywords: Stable isotopes, melting, structure, fluid, melt, spectroscopy

Importance of being salty: Elemental partitioning between melts and aqueous fluids and salinity of fluid inclusions from subduction channels and mantle wedges

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In order to understand seawater recycling in subduction zones, we determine the salinity of natural fluid inclusions in harzburgites from the mantle wedge (Kawamoto et al., 2013, PNAS, Kumagai et al., 2014 CMP) and jadeitites from serpentine mélanges of Southwest Japan and Dominican Republic.

High-pressure and high-temperature experiments suggest that saline fluids can effectively transport large-ion-lithophile elements (Kawamoto et al., 2014, Earth Planets and Space) and carbonate (Newton and Manning, 2002, American Mineralogist). In natural specimens, subduction-zone fluids contain more or less amounts of salt. The salinity of aqueous fluids in the mantle wedge seems to decrease from trench side to back-arc side: from 5.1 wt% NaCl equivalent in harzburgite xenoliths of the Pinatubo, a frontal volcano of the Luzon arc, the Philippines [Kawamoto et al., 2013 Proc Natl Acad Sci USA] to 3.7 wt% NaCl equivalent in lherzolite xenoliths of the Ichinomegeta, a rear-arc volcano of the Northeast Japan arc [Kumagai et al., Contrib Mineral Petrol 2014]. Abundances of chlorine and H_2O in olivine-hosted melt inclusions also suggest that frontal basalts have higher Cl/H_2O ratios than rear-arc basalts in the Guatemala arc [Walker et al., Contrib Mineral Petrol 2003]. In addition to these data, quartz-free jadeitites contain fluid inclusions composed of aqueous fluids with 7 ±0.3 wt% NaCl equivalent and quartz-bearing jadeitite with 4.6 ± 1.2 wt% NaCl equivalent in supra-subduction zones in the Southwest Japan arc [Mori et al., 2015, International Eclogite Conference] and quartz-bearing jadeitites contain fluid inclusions composed of aqueous fluids with 4.3 ±1.3 wt% NaCl equivalent in Rio San Juan Complex, Dominica Republic [Kawamoto et al., 2015, Goldschmidt Conference]. Aqueous fluids generated at pressures lower than conditions for albite=jadeite+quartz occurring at 1.5 GPa, 500 °C may contain aqueous fluids with higher salinity than at higher pressures. All of these salinity data in natural fluid inclusions have values similar to or slightly greater than the value of seawater (3.5 wt% NaCl equivalent) and show decreasing salinity from trench to back-arc side in the mantle wedge and subduction channels.

Keywords: saline fluids, aqueous fluids, subduction zone, fluid inclusions, mantle wedge, magma

Serpentinized oceanic mantle and global water budget

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Hydration of oceanic mantle can occur along outer-rise faults that relate to the plate bending at close to the trench (Faccenda et al. 2009). This contributes an additional source of water into the Earth’s interior, which might have larger water flux than that transported by hydrated oceanic crust. Recent seismic reflection survey has shown that seismic velocity in the oceanic lithosphere decreases at where bending-related faults are observed (e.g., Ranero et al. 2003; Fujie et al. 2013). Although these seismic data is not enough to image what extent of hydration occurs along the outer-rise faults, we modeled the thickness of serpentinization based on fluid percolation. When the reaction kinetics is much faster than the fluid access to the reaction front, the reaction rate is controlled by permeability through the hydrated layer (Macdonald and Fyfe 1985). Using laboratory measured permeability, the reaction thickness of serpentinization is estimated as thick as 18 km for a period from the initiation of outer-rise fault to the trench axis assuming a plate velocity of 10 cm/year. If outer-rise faults occur at depths shallower than 12 km, subduction water flux is estimated to be 2.5 x 10^{12} kg/year by hydrated oceanic mantle lithosphere, which is approximately twice as larger as that carried by hydrated oceanic crust. Since the subduction water flux is markedly larger than the output flux through magmatic degassing, the amount of present-day ocean is now decreasing and might be disappeared within 100 million years.

Keywords: serpentinite, oceanic mantle, water budget

Experimental investigations into the fate of water in Earth's transition zone

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The transition zone differs from the upper or lower mantle in that its major constituent minerals wadsleyite and ringwoodite can accommodate a significant amount of hydrogen in the crystalline structures. Translated into water storage capacities, hydrous wadsleyite or ringwoodite may contain several weight percent water, whereas the dominant minerals above or below the transition zone are nominally dry. The recent discovery of hydrous ringwoodite brought to the surface by a super-deep diamond indicates that transition zone is likely a sub-surface hydrosphere containing a comparable amount of water to the surface oceans. As a result of large contrast in water storage capacities, a wet transition zone is expected to dehydrate and form partially molten layers near its upper and lower boundaries when the interfaces are pushed downwards by descending slabs or upwards by rising plumes. Convection-induced dehydration of a wet transition zone may explain the seismically detected low-velocity zones near 410 and 660 km depths. In this study we test the hypothesis that dehydration is not limited to the interfaces but can take place in the interior of the transition zone following incipient melting of carbon-bearing materials that are carried to mid-mantle by subducted slabs. Experiments have been conducted using a multi-anvil apparatus to investigate the partitioning of hydrogen between hydrous wadsleyite or ringwoodite and coexisting carbonates or iron-carbon mixture at relevant high pressures and high temperatures. The results will be applied to understand the sources and sinks of water in Earth's transition zone and to elucidate the connections between the surficial and internal hydrospheres.

Keywords: transition zone, water, hydrous wadsleyite and ringwoodite, carbonates, iron-carbon mixture, melting

“Hydroxylation spectroscopy” of olivine tested on synthetic forsterite

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Olivine $(Mg,Fe)_2SiO_4$, the most abundant phase in the upper mantle, can incorporate a few ppm to tens or even hundreds of ppm of water as hydroxide anions in its structure. Even at such low concentrations, the presence of H^+ in the structure of olivine has a profound influence on its physical properties and, consequently, geologic processes such as mantle convection and partial melting. The incorporation of H^+ in olivine is mediated by a variety of hydrous point defects, related to Si^{4+} and Mg^{2+} vacancies, or coupled substitution with Ti^{4+} or trivalent cations (*e.g.*, Al^{3+}). These different types of hydrous point-defects can be fingerprinted using infrared spectroscopy. The point defect chemistry of olivine depends on parameters such as silica activity or oxygen fugacity, which are inherent to the last equilibrium conditions of the olivine. If the relaxation of the high-temperature point defect structure is slow compared to the rapid diffusion of H^+ into the crystal, then “decorating” the existing point-defect structure of an olivine by experimentally diffusing H^+ into it potentially makes its point-defect structure visible to identification using infrared light, thus revealing information about its geologic history. Here we present experimental results to test whether we can illuminate the pre-existing point defect structure of synthetic forsterite (Mg_2SiO_4) prepared under controlled conditions of temperature, silica activity and oxygen fugacity, as a first step towards seeing how effective this technique of “hydroxylation spectroscopy” may be in illuminating the point defect chemistry of natural mantle olivine crystals. Experiments were performed with cubes of synthetic forsterite in a piston cylinder apparatus. The forsterite cubes were annealed at temperatures ranging between 1100 and 1500 °C for 8 days, in contact with Forsterite-Enstatite (Fo-En) or Forsterite-Periclase (Fo-Per) silica activity buffers. Annealed and un-annealed cubes were then loaded in silver capsules along with liquid water and a combination of silica activity and oxygen fugacity buffers. Hydroxylation of the cubes was done at 900°C and 1.5 GPa. Unpolarized and polarized infrared spectra were acquired along the principal axis of the crystals, along profiles of a few hundred micrometers. From those spectral profiles, diffusion coefficients were quantified and the diffusion mechanisms inferred, using the unique infrared signature of each type of defect.

Results show that H^+ diffuses faster than expected in [Si] vacancies, such that this mechanism may contribute as much as H^+ diffusion in [Mg] vacancies to the global diffusion of “water” in Forsterite. The hydroxylation experiments further allow us to assess how the initial annealing conditions of the crystals influence the diffusion mechanism of H^+.

Keywords: Olivine, Water, Diffusion, Hydroxylation, Infrared spectroscopy

Hydrogen incorporation in olivine

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The main silicate phases of the Earth's upper mantle, namely olivine, pyroxenes and garnet, do not have hydrogen as an essential component of their crystal structures, but they can contain geologically significant amounts of hydrogen as a trace element, substituting by point-defect mechanisms. In the context of hydrogen storage, these phases have therefore become known as "Nominally Anhydrous Minerals" or NAMs. The good correlations of H with incompatible trace elements like the light Rare Earth Elements (e.g., Ce) in suites of mid-ocean-ridge and ocean-island basalts (MORBs and OIBs) confirms the essentially trace-element-like behaviour of H. The H in NAMs occurs bonded to the oxygen anions (O^{2-}) in their crystal lattices, forming hydroxyl species (OH^-), and charge-balanced by cation vacancies with or without the coupled substitution of cations with different charge to those in the stoichiometric crystals. The presence of the OH^- anions is readily detected by infra-red spectroscopy, due to the good absorbance of the O-H stretching modes in the infra-red. Moreover, the O-H stretching modes are sensitive to next-nearest-neighbour effects, which may be used to deduce the nature of the H substitution mechanisms.
For Mg_2SiO_4-rich olivine, the most abundant phase in the upper mantle, experiments show that four different substitution mechanisms are commonly encountered, each identifiable by its characteristic infra-red fingerprint: those associated with Mg and Si vacancies, with 3+ cations, and with Ti^{4+}. Note that other H substitution mechanisms in olivine may exist under special circumstances, e.g., in olivines containing boron. The four main substitution mechanisms can be represented by the four equilibria:
$H_2O + Mg_2SiO_4(ol) = Mg\underline{ov}SiO_2(OH)_2(ol) + MgO$ (Mg-vacancies)
$2\ H_2O + Mg_2SiO_4(ol) = Mg_2\underline{tv}(OH)_4(ol) + SiO_2$ (Si-vacancies)
$0.5\ H_2O + Mg_2SiO_4(ol) + R^{3+}O_{1.5} = R^{3+}\underline{ov}SiO_3(OH)\ (ol) + 2\ MgO$ (trivalent)
$H_2O + MgO + TiO_2 = MgTi\underline{tv}O_2(OH)_2(ol)$ (titanoclinohumite point defect, or TiPD)
where $\underline{ov}$ and $\underline{tv}$ stand for octahedral and tetrahedral cation-site vacancies, respectively.
The H concentrations controlled by each of these four equilibria will in principle respond differently to temperature and pressure, and to chemical environment, specifically, to the activity of silica (a_{SiO2}), and the availability of trivalent cations and Ti. Importantly, the stoichiometry of the substitution mechanisms implies that they may also respond differently to $f(H_2O)$, if short-range ordering maintains the local charge balance implied by the substitution formulae; such short-range ordering seems required by the distinctiveness of the infra-red fingerprints. With short-range order, the concentration of H associated with trivalent cations would depend on $f(H_2O)^{1/2}$, with Mg-vacancies and TiPD on $f(H_2O)$, and with Si-vacancies on $f(H_2O)^2$. New experiments on H incorporation in $Mg_2SiO_4(ol)$ doped with Sc and Ti at 15 kb and 1050ºC, with $f(H_2O)$ controlled at different values using H_2O-NaCl mixtures, confirm this hypothesis. This means that results from experiments at high $f(H_2O)$ (e.g., with $p(H_2O) = P_{total}$) cannot be applied directly to natural situations where $p(H_2O) << P_{total}$.The different substitution mechanisms are also associated with very different diffusion rates of H through olivine, and it is likely that they affect physical properties differently too.

Keywords: Hydrogen, Olivine, Nominally Anhydrous Minerals, Mantle

Hydrogen mobility in transition zone silicates

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Hydrogen defects in mantle silicates adopt a variety of charge-balanced defects, including V_{Mg}''+2(H*), V_{Si}''''+4(H*), and V_{Si}'+(Mg+2H*). Constraining the defect mechanism experimentally can be quite difficult, as it relies almost entirely on vibrational spectroscopy whose interpretation can often be controversial. Here we use a computational alternative: we study the above-mentioned defect mechanisms using molecular dynamics simulations based on the density-functional theory, in the VASP implementation. We perform isokinetical NVT simulations at 2000 and 2500 K using supercells containing 16 equivalent formula units of Mg_2SiO_4.

Our results show that temperature has a tremendous effect on mobility. H is significantly more mobile when incorporated as V_{Mg}''+2H* defects than as hydrogarnet defects and that V_{Mg}''+2H* defects are more mobile in wadsleyite than ringwoodite. This result is the opposite from the proton conductivity inferences of Yoshino et al. [2008] and Huang et al [2006], as well as the observed increase in electrical conductivity with depth through the transition zone [e.g. Kuvshinov et al, 2005; Olsen 1998].

Over the simulation time of several tens of picoseconds the H travel over several lattice sites. However, during its path it spends a considerable amount of time pinned in the defect sites. The lowest mobility is for the V_{Si}''''+4(H*) defect, where the H atoms remain inside the octahedron from which they replaced the Si.

Keywords: diffusion, molecular dynamics, mantle silicates

Sound velocities of delta-AlOOH up to lowermost mantle pressures; Implications for the seismic anomalies in deep mantle

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It is widely recognized that the presence of water in the deep Earth’s interior, which may be transported to such depths by various hydrous minerals in subducting slabs, can significantly affect the physical and rheological properties of the mantle. Most hydrous minerals become thermodynamically unstable under the pressure-temperature conditions corresponding to the upper part of the upper mantle (e.g., Ohtani, 2006). However, recent experimental data indicate that the hydrous mineral delta-AlOOH can be stable throughout the lowermost mantle (Sano et al., 2008; Ohira et al., 2014; Ohtani et al., 2014). This phase is, therefore, a possible carrier and host of water in the deep mantle. To uncover the physical properties of delta-AlOOH under deep mantle pressure conditions, we have conducted high-pressure acoustic wave velocity measurements of delta-AlOOH by using Brillouin spectroscopy combined with high-pressure Raman spectroscopic measurements in a diamond anvil cell up to pressures of 134 GPa. There is a precipitous increase by ~14% in the acoustic velocities of delta-AlOOH from 6 to 15 GPa, which suggests that pressure-induced O-H bond symmetrization occurs in this pressure range. The best fit values for the high-pressure form of delta-AlOOH of K_0 = 190 (2) (GPa), G_0 = 160.0 (9) (GPa), $(\partial K/\partial P)_0 = K_0'$ = 3.7 (1), and $(\partial G/\partial P)_0 = G_0'$ = 1.32 (1) indicate that delta-AlOOH has a 20–30% higher V_S value compared to those of the major constituent minerals in the mantle transition zone, such as wadsleyite, ringwoodite, and majorite. On the other hand, the V_S of delta-AlOOH is ~7% lower than that of bridgmanite under lowermost mantle pressure conditions. By comparing our results with seismic observations, we can infer that delta-AlOOH could be one of the potential causes of a positive V_S anomaly observed at ~600 km depth beneath the Korean peninsula and a negative V_S jump near 2800 km depth near the northern margin of the large low-shear-velocity province beneath the Pacific.

Keywords: delta-AlOOH, Brillouin scattering, seismic anomaly, transition zone, lower mantle

In-situ observation of hydrogen-bond symmetrization in δ-AlOOH and its isotope effect

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Hydrogen bond is unique compared to the other covalent bond that makes a framework of minerals. Generally hydrogen bonds covalently to one side of oxygen while it forms hydrogen bond with the other side of oxygen, which is longer and soft bond. Applying pressure to this asymmetric geometry induces the decrease of O...O distance and results in various interactions with surrounding atoms. These changes are unquenchable to ambient pressure thus *in-situ* neutron diffraction experiment is indispensable to shed the light on hydrogen bond under high-pressure.
Aluminus hydrous mineral δ-AlOOH [1] has a strong hydrogen bond in its distorted rutile type structure at ambient conditions. Its stability field expands in wide pressure and temperature range, from 18 GPa to 134 GPa, and up to 2300 K [2] and considered as an important water carrier into the lower mantle. Ab-initio calculations pointed out that the hydrogen locates at the center between two oxygen atoms at high-pressure, which is so-called “symmetrization” of hydrogen bond [e.g. 3]. It is also suggested that the increase of bulk modulus is induced by the symmetrization. Subsequent X-ray diffraction study found that the bulk modulus increases at around 10 GPa for δ-AlOOH and 12 GPa for δ-AlOOD. Neutron diffraction study was conducted to 9.2 GPa but the hydrogen bond remains asymmetric in this pressure range [4].
To observe pressure-induced hydrogen-bond symmetrization directly, we conducted high-pressure neutron diffraction experiments to 18.1 GPa. The samples of δ-AlOOH and δ-AlOOD were synthesized at 18 GPa and 800-900 °C using a multi-anvil press. The synthesized sample and deuterated methanol-ethanol pressure-transmitting medium were loaded into a TiZr gasket in a Paris-Edinburgh press. Neutron diffraction patterns were corrected at the high-pressure neutron diffractometer “PLANET” in the MLF, J-PARC. The crystal structure including a hydrogen and deuterium position was refined by Rietveld method.
In δ-AlOOH, the disappearance of 021 reflection was observed at high-pressure. This observation can be attributed to the transition from the space group of $P2_1nm$ with asymmetric hydrogen bond to that of *Pnnm* with disordered or symmetric hydrogen bond. The transition pressure of 8.4 GPa is consistent with our previous single crystal X-ray diffraction experiment. On the other hand the transition pressure of δ-AlOOD was determined to be 12.1 GPa, which is higher than that of δ-AlOOH. The O...O distance of hydrogen bond decreases significantly compared to other O...O distances below the transition but it becomes less compressible above the transition pressure. The result reveals that the small change of hydrogen position can induce the significant change of compression behavior. To discuss the detail hydrogen distribution in the *Pnnm* structure, the difference Fourier map was obtained from the difference between the observed diffraction pattern and the refined model without hydrogen. The result will be presented in the paper.

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Keywords: hydrogen bond, neutron diffraciton experiment, high pressure, isotope effect

Hydrogen solubility into Fe-alloys under high pressure

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Hydrogen, the most abundant element in the solar system, is known to incorporate into Fe and form FeH_x above 3 GPa. The solubility of H in Fe is closely linked to light element in the terrestrial core and H reservoir in the planet interiors. In order to understand more realistic case of H in planet interiors, H solubility into Fe-alloys (such as Fe-Si, Fe-C, and Fe-S) needs to be clarified.

In this study, we have performed in situ X-ray diffraction measurements combined with Kawai-type multianvil press under high pressures and temperatures to study H solubility in FeSi and Fe3C. H solubility can be estimated from a volume expansion associated with hydrogen incorporation into metal. The lattice volumes and phase relations of FeSi-H and Fe3C–H systems were measured up to 19 GPa and 1973 K.

H starts to dissolve in FeSi and form $FeSiH_x$ (x=0.07-0.22) above 10 GPa, suggesting that presence of Si in metal increases the minimal pressure for H incorporation. H incorporation into Fe3C does not occur and H is unlikely to coexist with C in Fe-alloy up to 14 GPa (Terasaki et al. 2014). Therefore, hydrogenation pressures of Fe-alloys are different from that of pure Fe and more pressure is required for H incorporation into the Fe-alloy core.

Keywords: Hydrogen, Fe-alloy, core