Impact of volatiles on the processes of formation and evolution of the Earth's interior

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Mon. Apr 28, 2014 4:15 PM - 5:45 PM  411 (4F)

Characterization of the processes that govern the behavior, budget, and recycling of volatiles in the Earth's interior is fundamental to our understanding of the formation and evolution of the solid Earth, its oceans, and atmosphere. In the proposed session, we will focus on theoretical, experimental, and observational characterization of solubility and solution mechanisms of C-O-H-N-S volatiles in molten and crystalline materials and of oxide components in C-O-H-N-S fluid in the pressure, temperature, composition and redox range of Earth's past and current interior. The major session foci will be:

2. Characterization of structure and properties in silicate-C-O-H-N-S melt, mineral, and fluid systems via theoretical modeling and high-temperature/-pressure experimental studies.
3. Experimental characterization, at high temperature and pressure, of fractionation of components, compounds and isotopes in the C-O-H-N-S system between minerals, melts, and fluids.
4. Element complexing in individual phases, interaction between silicate and trace and minor elements in fluids and melts at high temperature and pressure.
5. Examine the principles on which to quantify property behavior and its application to natural processes that include fluids and melts.

Hydrogen positions in hydrous ringwoodite determined by pulsed neutron powder diffraction

Keywords:ringwoodite, neutron diffraction, Rietveld refinement

The transition zone in the Earth's mantle has been considered potentially large water reservoir. It was experimentally evidenced that its main constituent minerals can uptake significant amount of water as hydroxyl groups in their crystal structures. The ringwoodite [(γ-Mg,Fe)₂SiO₄] is one of the high pressure polymorph of olivine, which is the most major phase in the lower part of the transition zone, between 525 to 660 km in depth. It was reported that ringwoodite can incorporate up to 2.6 wt.% of water (Kohlstedt et al., 1996). The hydration of ringwoodite strongly affects its physical and chemical properties such as electrical conductivity, compressibility and seismic velocities. However, crystallographic sites of hydrogen and its incorporation mechanism are still unclear mainly due to insensitiveness of X-ray probe for hydrogen. The previous studies of its structure refinement by X-ray diffraction demonstrated that hydrous ringwoodite has cubic spinel structure with Fd-3m space group (Kudoh et al., 2000; Smyth et al., 2003). Here we applied neutron diffraction for hydrous ringwoodite for the first time to analyze its hydrogen positions. Deuterated ringwoodite powder samples were synthesized at 1300 °C and 18 GPa for 5 minutes using a scaled-up Kawai-type multi anvil apparatus. The
run products were evaluated by micro-focused X-ray, Raman spectroscopy and powder X-ray
diffractometer to confirm their purity. Neutron powder diffraction patterns were taken at BL-19
(TAKUMI) at Materials and Life Science Experimental Facility, J-PARC. The two representative
deuterated ringwoodite samples were with identical composition mixed and measured together in a
sample holder made of TiZr "null" alloy. The obtained diffraction pattern has been analyzed by Rietveld
refinement using the "Z-Rietveld" code in order to determine positions and site occupancies of deuterium
atoms in the ringwoodite structure. We can propose two possible models for the deuterium atomic
positions, 96g and 192i. These refined models were given with almost identical R factors. They also gave
similar site occupancies and temperature factors for the elements except for the deuterium. However, in
terms of deuterium temperature factor, the 192i model is more preferable than the 96g model. The
refinement results also showed that the (Mg+Fe)/Si ratio is lower than the ideal ratio of dry
ringwoodite [(Mg+Fe)/Si = 2.0] while Si in T sites are fully occupied, which demonstrates that deuterium
only substitutes Mg and Fe in M sites and Si in T sites is not affected. References: [1] Kohlstedt, et al.,