Japan Geoscience Union Meeting 2014
(28 April - 02 May 2014 at Pacifico YOKOHAMA, Kanagawa, Japan)

SMP47-13 Room:422 Time:May 1 12:15-12:30

Structure analysis of deuterated brucite at pressures to 3 GPa by pulsed neutron powder diffraction

OKUCHI, Takuo[1*] ; TOMIOKA, Naotaka[1] ; PUREVJAV, Narangoo[1] ; HARJO, Stefanus[2] ; ABE, Jun[3] ; WU, Gong[2]

[1]Institute for Study of the Earth's Interior, Okayama University, [2]Japan Atomic Energy Agency, [3]CROSS Tokai

Atomic-scale structures around hydrogen atoms in hydrous minerals may significantly change with increasing pressure, which affect thermodynamic stability, optical properties (Raman, IR, etc.), and transport phenomena of the relevant minerals. To directly observe such structure change around hydrogen atoms, we have conducted neutron diffraction experiments of deuterated brucite at high pressures to 2.8 GPa, using a high-resolution neutron powder diffractometer recently installed at J-PARC Materials and Life Science Experimental Facility. To discriminate subtle structure change of deuterium site positions with increasing pressure, the quality of observed diffraction patterns has been considerably improved from the corresponding previous studies by adopting a new-type experimental apparatus and facility. A newly-designed opposed anvil cell apparatus optimized for the pulsed neutron beam (Okuchi et al., High Pressure Research, 33, 777, 2013) was effectively coupled with the time of flight diffractometer TAKUMI, which was designed to have the resolution of delta-d / d ˜0.3% along with moderately-intense beam and low background (Harjo et al., Materials Science Forum, 524, 199). We used single crystal diamond anvls with culet diameter of 2 mm for sample compression along with deuterated glycerine pressure medium. The combination gives very high neutron transparency as well as high resolution to enable acurate structure refinements of tiny sample volume of the order of less than 1 mm^3. Through Rietveld refinements of the observed patterns, tilting of all OD dipoles in the compressed brucite toward one the three nearest-neighbor oxygen anions in the brucite structure was confirmed to be substantial at the observed pressure regime, suggesting the formation of pressure-induced hydrogen bonding. Therefore, at lower crust and mantle wedge conditions, this pressure-induced bonding may play an important role to constrain hydrogen into the relevant hydrous minerals.

Keywords: hydrogen, brucite, high pressure, neutron diffraction