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

SMP47-P02 Room:Poster Time:May 1 18:15-19:30

Thermal expansion of $Ca(OD)_2$ at high pressure

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$Ca(OH)_2$ is one of the important hydrous minerals to understand structural behavior at high pressure and high temperature, because this type of structure is a building unit in more complex hydrous phases such as chondrodite. It is surprising that only a few previous researches can be found on crystallography of $Ca(OH)_2$ in the conditions of simultaneously high pressure and high temperature. We gave an oral presentation about some preliminary results in this conference last year. We have continued to analyze the data carefully and will add some new information.

Deuterated samples were prepared via hydrothermal treatment with CaO fine powders and excess D_2O water in a Teflon lined stainless steel autoclave at 493 K for 4 days. After the hydrothermal treatment was completed, precipitates were filtered out, washed with D_2O water, and then dried at 383 K under vacuum for 3 hours. The products were confirmed to have the CdI2-type structure by conventional powder X-ray diffraction measurements and were checked to be deuterated by IR absorption spectra. Synchrotron X-ray diffraction experiments were performed at the beamline AR-NE5C, KEK, Japan in order to obtain cell parameters of $Ca(OD)_2$ at various P-T conditions from 2-4 GPa and 300-800 K. TOF neutron powder diffraction measurements of $Ca(OD)_2$ were carried out from 300 to 773 K at high pressure at the PLANET beamline in J-PARC, Japan. Pressure was estimated by comparing unit cell parameters with those obtained by synchrotron experiments.

All our TOF data obtained include only $Ca(OD)_2$ peaks and no peaks from sample surrounding materials such as ZrO_2 pressure medium, graphite furnace and WC anvils could be detected owing to radial collimators equipped with the 6-ram pressure apparatus (Atsuhime). The detailed structure parameters such as lattice parameters and atomic coordinates could be reasonably refined by the Rietveld method by using a program GSAS. It is an interesting result that thermal expansion along the *c*-axis seems to be suppressed at high pressure comparing to that at ambient pressure. Mechanism of the thermal expansion of $Ca(OD)_2$ at high pressure will be discussed.

Keywords: portlandite, thermal expansion, high pressure, synchrotron X-ray diffraction, TOF neutron diffraction