Japan Geoscience Union Meeting 2010
(May 23-28 2010 at Makuhari, Chiba, Japan)

SMP056-P09 Room: Convention Hall Time: May 23 17:15-18:45

Refinement of hydrogen positions in super B at 1.0 and 3.5 GPa using ME analysis with single crystal diffraction data

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Hydrogen bonding has unique properties in the view of material science. Under high-pressure and high temperature (-10 GPa, - 1000C) conditions, hydrous minerals such as dense hydrous magnesium silicate minerals (DHMS), which have hydrogen bonding in its structure, are stable because of the special property of the bonding. It is important to investigate the behavior of hydrogen bonding under high-pressure for understanding its unique property. In this study, using ME (Maximum Entropy Method) analysis with single crystal X-ray diffraction data, we tried to refine hydrogen positions of DHMS phases (in this talk, super hydrous phase B) under high-pressure conditions (at 1.0 GPa and 3.5 GPa).
Sample (sup_B) was synthesized at 20 GPa and 1000 C kept 4 hours using the Kawai type multi-anvil apparatus installed in Gakushu-in University. Single crystal (80 x 80 x 40 um3) of sup_B was used for X-ray diffraction measurements at BL-10A, PF, KEK. The used wavelength was 0.6 493 A. The intensity data sets under high-pressure conditions were measured using the four-circle diffractometer with a DAC. After Lp, background and absorption corrections were applied for all measured data, structure refinements were conducted using SHELX97. Anisothermal temperature factors for all atoms except hydrogen were applied. PRIMA (Dilanian and Izumi, 2002) was used for ME analysis with the phases based on the results from structural refinements.
For the ambient conditions data set, the electron density corresponded to hydrogen position was observed. Then for high-pressure data, results from D-fourier and ME analyses, electron density distribution of hydrogen was observed. For 1.0 GPa data sets, hydrogen positions and isothermal temperature factors of super hydrous phase B could be refined. The determined O-H distance was 0.86(9) A. This result showed that even though under high-pressure conditions, when we obtain very precised X-ray intensity data sets, hydrogen positions should be refined.

Keywords: single crystal structure analysis, hydrous minerals, high-pressure, hydrogen posiiton