Estimation for hydrogen positions in hydrous minerals under high-pressure using MEM 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 MEM (Maximum Entropy Method) analysis with single crystal X-ray diffraction data, we tried to check whether hydrogen positions of DHMS phases under high-pressure conditions could be observed directly or not. In this talk, the X-ray intensity data set of super hydrous phase B (sup_B) at ambient conditions was used as the data set of high-pressure condition applying some limitations by assuming DAC measurements.

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 of sup_B was used for X-ray diffraction measurements. The intensity data set was measured using four-circle diffractometer. For MEM analysis, PRIMA (Dilanian and Izumi, 2005) was used. At ambient conditions, the electron density corresponded to hydrogen position was observed. Therefore, the hydrogen positions of minerals, which contain around 5.8wt% water, can be observed.