Neutron diffraction study of hydrogen bonding of delta AlOOD at high pressure

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Delta-AlOOH is a high-pressure polymorph of diaspore (alpha-AlOOH). The structure is similar to CaCl2-type SiO2 which is a high-pressure polymorph of stishovite; edge-sharing Al-O octahedra make single-chain along c-axis. This hydrous phase is remarkable for strong hydrogen bond suggested both short O-H...O length and broad peak at low frequency of raman spectra. First principals calculations also showed hydrogen bond of delta AlOOH to be symmetric. However, the transition pressure of asymmetric to symmetric bond is vary; Tsuchiya et al. (2002) suggest that transition occurs at 28 GPa whereas Panero and Stixrude (2004) argued that symmetric hydrogen bond is stable at ambient pressure. To investigate the hydrogen position and hydrogen bond behavior at the high pressure, we conducted the neutron diffraction experiments of delta-AlOOD.

Time-of-flight neutron diffraction study was performed at the PEARL high pressure facility of ISIS at Rutherford Appleton Laboratory. Delta-AlOOD was synthesized from deuterated bayerite starting material at 18 GPa and 900 C using multi anvil high pressure apparatus. For structure refinement at ambient condition, delta-AlOOD was loaded into the vanadium can. High pressure diffraction data was corrected using an opposed-anvil Paris-Edinburgh cell. Sample was loaded into the Ti-Zr gasket and deuterated MeOD/EtOD was added as pressure medium. Pressure was calculated from refined unit cell volume using equation of state of delta-AlOOH. Data was corrected up to 90 tons and any significant broadening was not observed. The data of neutron diffraction experiment will provide understanding for the hydrogen bonding property of delta-AlOOD at high pressure.