Powder neutron diffraction and Raman spectra for bayerite at high pressure

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Minerals of the alumina-water system, which have the composition of Al(OH)3, are gibbsite [gamma-Al(OH)3], bayerite [alpha-Al(OH)3], nordstrandite [beta-Al(OH)3] and doyleite [no alphabetical notation]. These Al(OH)3 polymorphs consist of Al octahedral layer parallel to (001). Among them, it is known that gibbsite undergoes a phase transition at 2-3 GPa, and the crystal structure of the high pressure phase of gibbsite [named as eta-Al(OH)3] was solved by in-situ single crystal X-ray diffraction (Komatsu et al., 2006; this meeting). On the analogy of the structural similarity between the Al(OH)3 polymorphs, it is likely that a pressure-induced phase transition of other Al(OH)3 polymorphs could be possible. However, little is known about the phase transition except for gibbsite. In this study, powder neutron diffraction and Raman spectra for bayerite were measured at high pressure.

A bayerite powder sample was loaded into a vanadium can to measure at ambient pressure and was loaded between the opposed sintered-diamond anvils of a Paris-Edinburgh high-pressure cell on the on the PEARL/HiPr diffractometer at ISIS. The sample was in a soft-metal-encapsulated (SME) gasket consisting of a null-scattering Ti-Zr alloy with a 4:1 deuterated methanol as the pressure transmitting medium. Pressure was achieved by the application of load to the anvils by an in situ computer-operated ram. The neutron diffraction at ambient pressure could be refined by Rietveld method as coded in the General Structure Analysis System (GSAS). Data at high pressure obtained by 90 degree bank were corrected for the attenuation of the neutron beam by the cell and the anvils. The applied loads to the cell were 7, 18, 55, 80 tons. Because the obtained neutron diffractions at high pressure were rather weak and broadened, it was difficult to refine the structure with sufficient accuracy. Raman spectra for bayerite were taken at high pressure using DAC, and the results also show no phase transition at least up to 6.5 GPa.