Compression behavior of delta-AlOOH and implication to the hydrogen bond symmetrization at high pressure

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Pressure response of hydrogen bonds in dense hydrous minerals attracts great attentions in deep earth sciences. Compression may induce hydrogen bond symmetrization; hydrogen-bonded protons initially located at asymmetric positions relocate to the symmetric midpoints at higher pressure. The first experimental observation of the hydrogen bond symmetrization was reported for ice at 110 GPa (Aoki et al., 1996). Theoretical calculations predicted that delta-AlOOH and Phase D undergo hydrogen bond symmetrizations at 28 GPa and 40 GPa, respectively (Tsuchiya et al., 2002 and 2005). Furthermore, considerable (approximately 20 %) increase in bulk modulus associated with the hydrogen bond symmetrization was simulated.

In the present study, we tried to detect the hydrogen bond symmetrization of delta-AlOOH by measuring its compressibility precisely. Delta-AlOOH was synthesized at 18 GPa and 900 degree C for 1 hour using a Kawai-type high-pressure apparatus at Tohoku University. Powdered sample was loaded into diamond anvil cells with helium or neon pressure transmitting medium in order to achieve quasi-hydrostatic condition up to quite high pressure. Powder X-ray diffraction patterns were obtained at BL04B2, SPring-8 at pressures up to 60 GPa and room temperature. Generated pressure was calibrated by the ruby fluorescence method. With increasing pressure, lattice constant ratios; a/c, b/c and b/a initially decreased up to 15-20 GPa and then contrastingly increased at higher pressure. This result suggests some change in the compression mechanism. Furthermore, the bulk modulus increased 20 % at the transition pressure. Because this increase is consistent with the theoretical prediction, our observation suggests that the hydrogen bond symmetrization of delta-AlOOH occurred in the pressure range of 15-20 GPa.