In-situ observation of pressure-induced symmetrization of hydrogen bond in δ-AlOOH and HD isotope effect

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Applying a pressure to hydrous mineral changes the distance of two oxygen atoms of hydrogen bond and induces various interactions between hydrogen and surrounding atoms. The changes are unquenchable thus in-situ neutron diffraction that has advantages to locate the hydrogen position provides insights into how hydrogen affects on the physical properties of minerals at high pressure.

δ-AlOOH is a distorted rutile type hydrous phase and considered to be a solid solution with recently reported dense hydrous mineral phase H. Theoretical studies indicate that compression results in the symmetrization of hydrogen bond, in which hydrogen locates at the midpoint between two oxygen atoms [1]. X-ray study have found the change in compressibility at high-pressure, with an isotope effect on the transition pressure. The pressure where the bulk modulus increases was 10 GPa for AlOOH whereas 12 GPa in AlOOD [2].

To examine the pressure response of hydrogen bond in δ-AlOOH and its D/H isotope difference, we performed neutron diffraction experiments at high-pressure neutron diffractometer PLANET in MLF, J-PARC [3]. The diffraction patterns of δ-AlOOH with deuterated and natural isotope compositions were measured at several pressures to 16.7 GPa. The transition from $P2_1nm$ to $Pnnm$, which can be attributed to the disorder of hydrogen bond or the symmtrization was found at 12.1 GPa for δ-AlOOD, at the same pressure where the change in compressibility was reported. The significant shortening of O…O distance and hydrogen bond was observed to 12.1 GPa; however, the O…O distance remains almost constant above the transition pressure. In comparison with deuterated sample, hydrogen bond in AlOOH is found to be longer at the same pressure. This study reveals that slight change of hydrogen position can induce the increase of bulk modulus in δ-AlOOH at high pressure.

[1] Tsuchiya et al. (2002) *Geophys. Res. Lett.* **29**, 1909. [2] A. Sano-Furukawa (2009) *Am. Mineral.* **94**, 1255-1261.[3] T. Hattori et al. (2015) *Nucl. Instrum. Methods Phys. Res. A* **780**, 55-67