Pressure-induced stacking disorder and non-symmetric hydrogen bond in boehmite

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It has gradually been accepted that significant amount of 'water' can exist as hydrous minerals in the deep Earth, at least locally at subducting slab or mantle transition zone, from the observation of high-P and high-T experiments and diamond inclusions (e.g., Peacock (2000) Science, **248**, 329; Pearson *et al.* (2014) Nature, **507**, 221). Because the main rock-forming minerals in the deep Earth are oxide or silicate minerals, hydrogens in hydrous minerals are surrounded by oxygens, and they form O-H...O hydrogen bonds (H-bonds). At high pressure, H-bond symmetrization may occur owing to the shortening O...O distances, yielding the O-H and H...O distances are equivalent, so that H-bonds in hydrous minerals occurred under some depth could be symmetrized. However, there are only a few studies regarding the H-bond symmetrization in hydrous minerals (e.g., Tsuchiya et al. (2002) Geophys Res Lett, 29, 1; Sano-Furukawa et al. (2009) Am Mineral, **94**, 1255; Tsuchiya and Mookherjee (2015) Sci Rep, **5**, 15534), and little is known about the relation between H-bond symmetrization with compression and the physical property change. Here we show a structure variation of boehmite with increasing pressure observed by using in-situ x-ray/neutron diffraction methods and Raman spectroscopy under pressure, and first found that pressure-induced stacking disorder would prevent H-bond symmetrization.

Keywords: Boehmite, High Pressure, Stacking disorder

