Stability and thermos-elastic properties of iron oxide hydroxide: water transportation in the Earth's interior

*Akio Suzuki[1]

1. Department of Earth and Planetary Materials Science, Faculty of Science, Tohoku University

Hydrogen in the Earth’ s interior plays an important role in the Earth’ s interior, e.g., reduction of melting temperature and enhancing the deformation. Hydrogen is also a candidate of the light element in the core on the basis of melting experiments. Therefore, the stability and physical properties of hydrous minerals are fundamentally important. We found a high pressure polymorph of diaspore over 19 GPa and named δ-AlOOH (Suzuki et al., 2000). Crystal structure of δ-AlOOH was determined to be InOOH type with an orthorhombic unit cell. On the basis of the structural similarity between δ-AlOOH and a high pressure phase of SiO_2 with $CaCl_2$ structure, we estimated that δ-AlOOH is an important candidate of the water reservoir in the lower mantle.
A high pressure phase of iron oxide hydroxide, ε-FeOOH, has also an InOOH-related structure. Recently, high-pressure X-ray diffraction study of ε-FeOOH was carried out, and the pressure-volume-temperature (*P-V-T*) equation of state was determined (Suzuki, 2016). The *P-V-T* data up to 11 GPa and 700K fitted to a third-order Birch-Murnaghan equation of state yield: isothermal bulk modulus K_{T0} of 135(3) GPa; its pressure derivative K' of 6.1(9); $(\partial K_T/\partial T)_P$ of -0.05(2) GPa K^{-1}; a_0 of 2.6(7)×10^{-5} K^{-1} and a_1 of 1.0(3)×10^{-7} K^{-2}, where the volumetric thermal expansion coefficient is described as $\alpha_{0,T}=a_0+a_1\times(T\text{-}300)$.
Here we report the results of X-ray diffraction study on goethite. Experiments were performed by using a Kawai-type multi-anvil apparatus driven by a 700 ton uniaxial press on the station NE7A at PF-AR, a synchrotron radiation facility in KEK, Tsukuba, Japan. Powder X-ray diffraction data were collected by the energy-dispersive method using a Ge-SSD detector at a fixed diffracted angle 2 theta of 6.0 degree. Goethite (α-FeOOH) is stable at ambient condition. We observed transformation to ε-FeOOH at 7.8+-0.5 GPa and 873K. The reduction of volume by the transformation was about 3.5%. The *P-V-T* data of goethite were collected up to 7.55 GPa and 600 K. Fitting the volume data to the third-order Birch–Murnaghan EoS yielded an isothermal bulk modulus, K_0 of 85.9(15) GPa, and a pressure derivative of the bulk modulus, K', of 12.6(8). The temperature derivative of the bulk modulus, $(dK/dT)_P$, was –0.022(9) GPa K^{-1}. The thermal expansion coefficient a_0 was determined to be 4.0(5) ×10^{-5} K^{-1}.
Dobson and Brodholt (2005) proposed that the banded iron formation subducted to the core-mantle boundary and stagnated there. The banded iron formation contains iron oxide-hydroxide. Goethite (α-FeOOH) transforms to ε-FeOOH at high pressure. At the core-mantle boundary, ε-FeOOH may react with the core, and oxygen and hydrogen are partitioned. We estimate that iron oxide hydroxide can transport hydrogen to the deep interior and supply hydrogen to the outer core. Also wüstite may be formed at the core-mantle boundary.

Keywords: mantle, hydrous phase, water, core, core-mantle boundary, high pressure

