

In-situ Raman spectroscopy of ϵ -FeOOH under high pressures

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ϵ -FeOOH is one of crucial high-pressure hydrous phases in the Earth's mantle, and is isostructural to δ -AlOOH. A first principles calculation (Gleason et al., 2013) has indicated pressure-induced hydrogen bond symmetrization at 43 GPa, and spin transition of iron at 65 GPa. These transitions cause changes in physical properties, and knowledge of the transition changes can help us to understand the behaviors of hydrous phases under high pressure.

We present a first study of Raman spectroscopy of ϵ -FeOOH at high pressure and room temperature. The measured sample was polycrystalline ϵ -FeOOH, which was synthesized in advance from a powder of reagent grade 99 % α -FeOOH at the pressure-temperature condition of 8 GPa and 480 °C for 2 hour. Micro-Raman spectrometer NRS-4100TOR (JASCO Corporation), which has a laser with the wavelength 532 nm and power 50 mW installed in Tohoku University, was used to obtain Raman spectra. Symmetric diamond anvil cell with 300 μ m culet size was used to generate high pressure. The sample was loaded in the sample chamber of tungsten gasket with NaCl pressure medium. The pressure in the chamber was calculated by means of the ruby luminescence pressure scale (Dewaele et al., 2004).

Along compression, the frequencies of most of peak tops have positive pressure dependences but some peaks (298, 386, 698, and 1099 cm^{-1} at 15 GPa) changed the dependences to negative around 14 GPa. Above 15 GPa some peaks (197, 298, and 443 cm^{-1} at 15 GPa) disappeared and the others (364, 386, 549, 646, 698, and 1099 cm^{-1} at 15 GPa) jumped by frequency 10–30 cm^{-1} . This change around 15 GPa may correspond to the replacement of vibrational modes in Raman spectra of δ -AlOOH at the pressure of 5.6 GPa (Mashino et al., 2016), which indicates a hydrogen-bond related space-group transition from $P2_1nm$ to $Pnnm$ (Tsuchiya et al., 2008).

Reference:

Dewaele, A., Loubeyre, P., and Mezouar, M. (2004). Equations of state of six metals above 94 GPa. *Phys. Rev. B* **70**, 094112.

Gleason, A.E., Quiroga, C.E., Suzuki, A., Pentcheva, R., and Mao, W.L. (2013). Symmetrization driven spin transition in ϵ -FeOOH at high pressure. *Earth Planet. Sci. Lett.* **379**, 49–55.

Mashino, I., Murakami, M., and Ohtani, E. (2016). Sound velocities of δ -AlOOH up to core-mantle boundary pressures with implications for the seismic anomalies in the deep mantle. *J. Geophys. Res. Solid Earth* **121**, 595–609.

Tsuchiya, J., Tsuchiya, T., and Wentzcovitch, R.M. (2008). Vibrational properties of δ -AlOOH under pressure. *Am. Mineral.* **93**, 477–482.

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