Report for the Joint Use/Research of the Institute for Planetary Materials, Okayama University for FY2023

05/29/2024

Category: ☐International Joint Research ☑General Joint Research ☐Joint Use of Facility ☐Workshop

Name of the research project: Sound velocity measurements of hydrous mantle minerals: Synthesis by Kawai-type multi-anvil apparatus

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Research report:

1. Research purpose

As δ-(Al,Fe)OOH is considered to be one of the most important hydrous phases on Earth, remaining stable under the extreme conditions throughout the mantle (Duan et al., 2018). The presence of δ-(Al,Fe)OOH may strikingly affects the physical properties of Earth's interior, including melting, thermal and electrical conductivity, elasticity, and phase transition (Hsieh et al., 2020; Liu et al., 2017; Mashino et al., 2016; Ohira et al., 2021; Ohtani, 2005; Satta et al., 2021; Su et al., 2023; Su et al., 2021). To date, it still remains unclear how the presence of iron and temperature affect its stability and elastic properties at extreme conditions, especially across the spin crossover. Therefore, **the purpose of research is to clarify how the presence of iron and temperature affect the stability**

and elastic properties of δ-(Al,Fe)OOH at extreme conditions, especially across the spin crossover.

2. Conducted research

2.1 Raman spectra of δ-(Al,Fe)OOH were measured at high temperatures and pressures up to 650 K and 62 GPa;

2.2 Single crystal XRD of δ-($Al_{0.85}Fe_{0.15}$)OOH at high temperatures and pressures was performed up to 900 K and 58 GPa.

3. Research outcomes

3.1 The vibrational properties and/or spin transition of δ-(Al,Fe)OOH analyzed by Raman spectroscopy up to 62 GPa and 650 K

The Raman spectra of δ-AlOOH were measured at high pressure up to 51 GPa and 300 K using Ar as a pressure transmitting medium (Figure 1). The pressure dependence of the Raman shifts decreases at ~6 GPa, which should be attributed to the symmetrization of hydrogen bonds (Kuribayashi et al., 2014; Mashino et al., 2016; Sano-Furukawa et al., 2009). Similarly, the onset pressure of hydrogen bonds symmetrization is ~6.5 GPa for δ-($Al_{0.85}Fe_{0.15}$)OOH (Figure 2). Moreover, the spin crossover of δ-($Al_{0.85}Fe_{0.15}$)OOH is 33.4(17)-37.9(8) GPa determined by the new occurred Raman mode and pressure dependence of the Raman shifts (Figure 2). Representative Raman spectra and shifts of δ-($Al_{0.85}Fe_{0.15}$)OOH with increasing pressure at 300 and 500 K using neon (Ne) as a pressure transmitting medium are shown in Figure 3. The spin crossover of δ-($Al_{0.85}Fe_{0.15}$)OOH is 38.1(8)-42.7(7) GPa at 500 K. The onset spin crossover pressure at 500 K is about 5 GPa higher than that of 300 K. Further results at higher temperatures are being collected and analyzed.

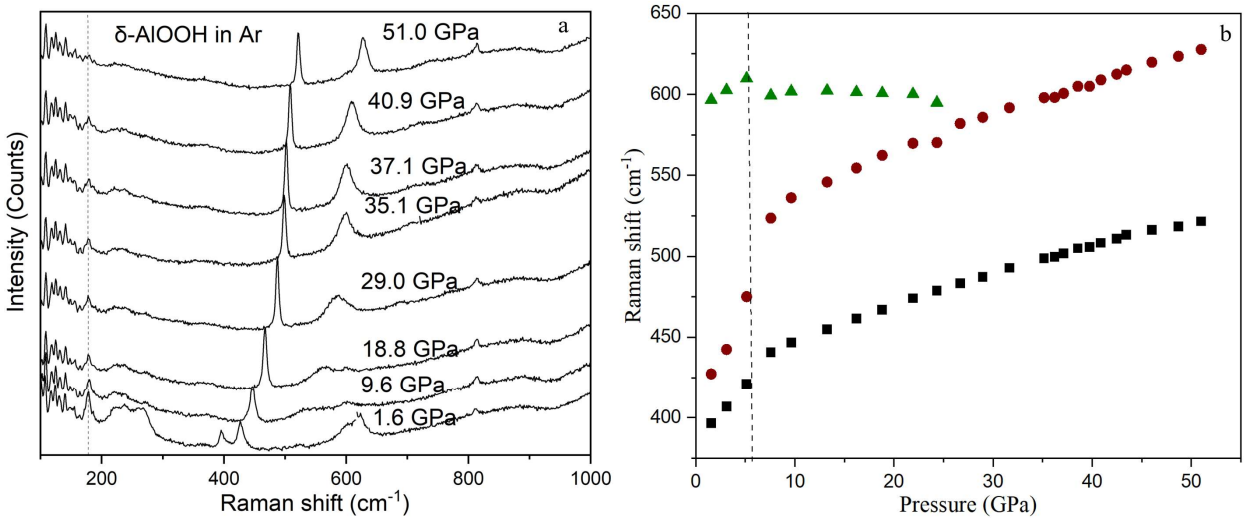

Figure 1. Representative Raman spectra and shifts of δ-AlOOH with increasing pressure. The dashed line represents the onset pressure of hydrogen bonds symmetrization.

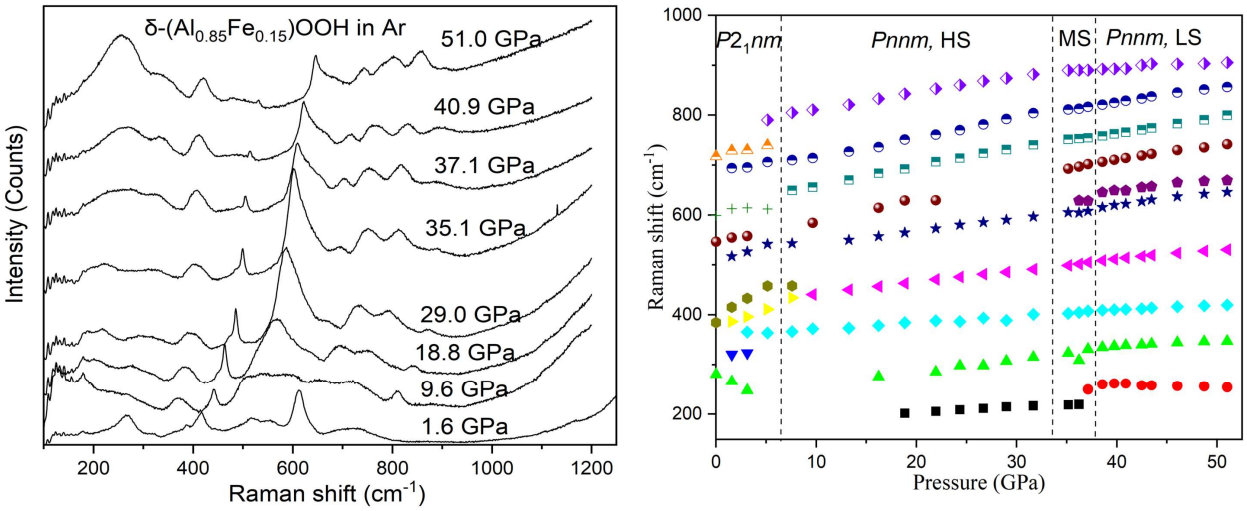

Figure 2. Representative Raman spectra and shifts of δ-$(Al_{0.85}Fe_{0.15})OOH$ with increasing pressure. The dashed line represents the onset pressure of hydrogen bonds symmetrization and spin transition of iron, respectively.

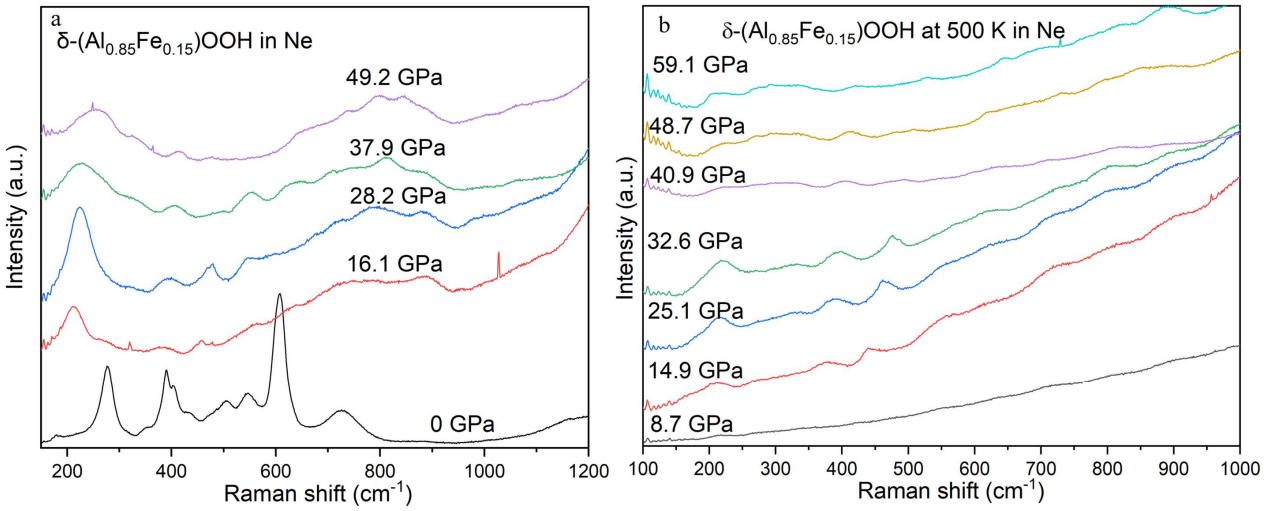

Figure 3. Representative Raman spectra and shifts of δ-$(Al_{0.85}Fe_{0.15})OOH$ with increasing pressure at 300 and 500 K using Ne as a pressure transmitting medium.

3.2 The unit cell parameters of δ-($Al_{0.85}Fe_{0.15}$)OOH determined by single crystal XRD up to 58 GPa and 900 K

Representative XRD spectra and unit cell parameters of δ-($Al_{0.85}Fe_{0.15}$)OOH with increasing pressure at 300 K are depicted in Figure 4. The pressure of the symmetrization of hydrogen bonds is ~8 GPa determined by single crystal XRD, which is ~2 GPa lower than previous study (Ohira et al., 2019). Moreover, the spin crossover of δ-($Al_{0.85}Fe_{0.15}$)OOH is 32-35 GPa, which is almost consistent with the results of 32-40 GPa (Ohira et al., 2019). The spin crossover range shifts to ~38-42 GPa at 500 K (Figure 5).

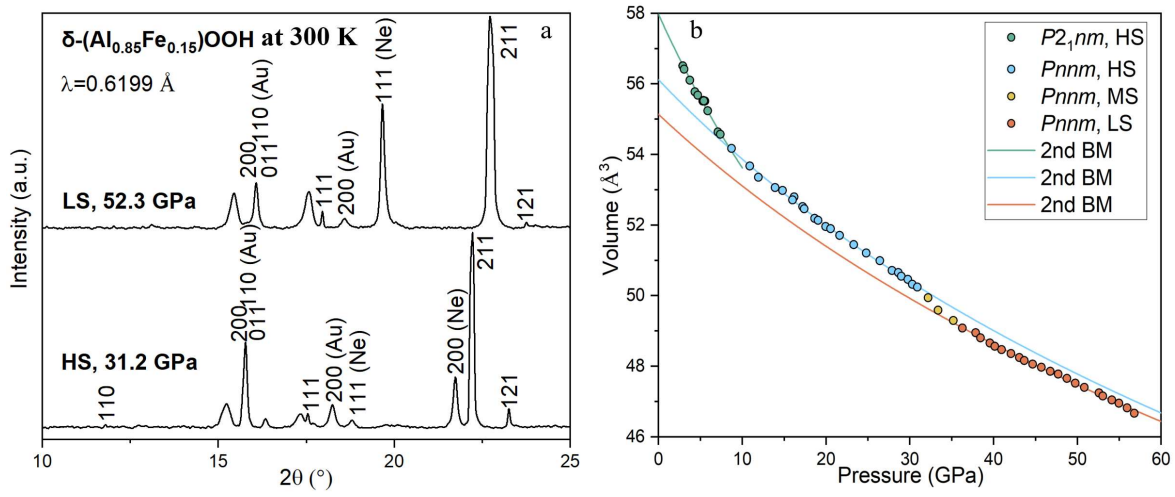

Figure 4. Representative XRD spectra of and unit cell parameters of δ-($Al_{0.85}Fe_{0.15}$)OOH with increasing pressure at 300 K.

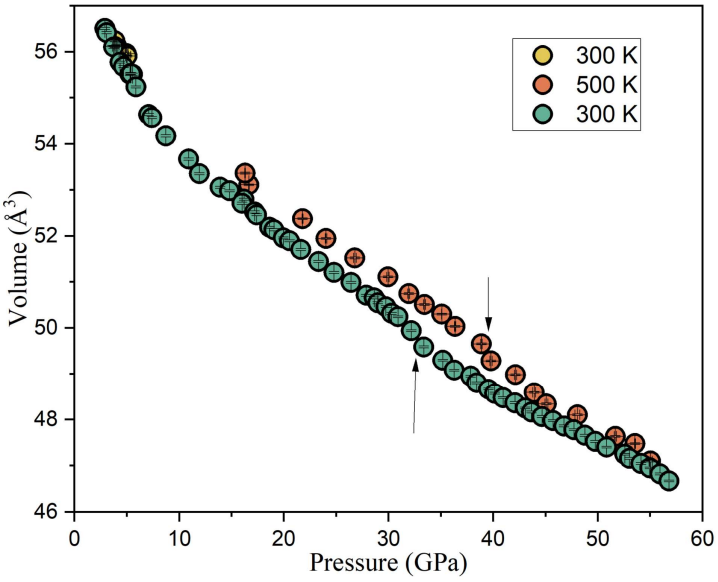

Figure 5. The unit cell parameters of δ-($Al_{0.85}Fe_{0.15}$)OOH with increasing pressure at 300 and 500 K.

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