# Report for the Joint Use/Research of the Institute for Planetary Materials, Okayama University for FY2024

05/28/2025

**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

Studying the physical properties of hydrated Al-bearing $CaCl_2$-type $SiO_2$ under high $P$–$T$ conditions relevant to the entire mantle is essential for understanding the deep water cycle, as well as the chemistry and dynamics of many geological processes.

## 2. Conducted research

2.1 Raman spectra of hydrated Al-bearing $CaCl_2$-type $SiO_2$ were measured at high temperatures and pressures up to 800 K and 65 GPa;

2.2 Single crystal XRD of hydrated Al-bearing $CaCl_2$-type $SiO_2$ was performed at high pressure up to 65 GPa at 300 K.

2.3 Single crystal IR of hydrated Al-bearing $CaCl_2$-type $SiO_2$ was performed at high pressure up to 50 GPa at 300 K.

## 3. Research outcomes

Synchrotron infrared spectroscopy experiments were conducted on two representative single-crystal (Al,H)-bearing $CaCl_2$-type $SiO_2$, $Si_{0.929}Al_{0.071}O_2H_{0.033}$ [$(Al_{7.1},H_{3.3})$-$SiO_2$] and $Si_{0.898}Al_{0.102}O_2H_{0.064}$ [$(Al_{10.2},H_{6.4})$-$SiO_2$] at high pressures up to 50 GPa at 300 K, respectively. the wavenumbers of OH mode increase monotonically again at ~30 GPa for $(Al_{7.1},H_{3.3})$-$SiO_2$ and ~27 GPa for $(Al_{10.2},H_{6.4})$-$SiO_2$, indicating the transition from disordered hydrogen to the hydrogen bond symmetrization states in $CaCl_2$-type $SiO_2$ (Fig. 1(a)). Raman spectroscopy independently confirms the hydrogen-bond symmetrization transition in (Al,H)-bearing $CaCl_2$-type $SiO_2$, consistent with synchrotron infrared observations (Fig. 1(b)). Synchrotron single-crystal XRD reveals that hydrogen-bond symmetrization markedly enhances the incompressibility of $CaCl_2$-type $SiO_2$ phase.

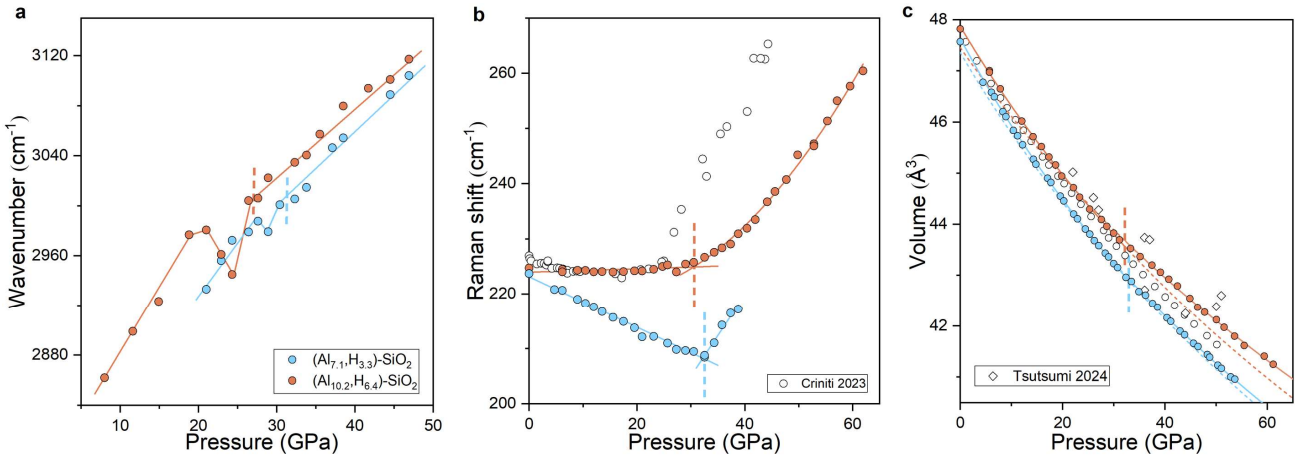


**Fig. 1| Hydrogen bond symmetrization of (Al,H)-bearing $CaCl_2$-type $SiO_2$ at high pressure and 300 K.**

Our high P-T Raman measurements reveal a pronounced temperature dependence for the hydrogen-bond symmetrization transition in (Al,H)-bearing $CaCl_2$-type $SiO_2$ (Fig. 2). As

temperature increases, the transition pressure decreases sharply for both compositions examined. The transition is identified by a reversal in the pressure dependence of the $A_{g1}$ Raman mode, consistent with the signature observed at 300 K.

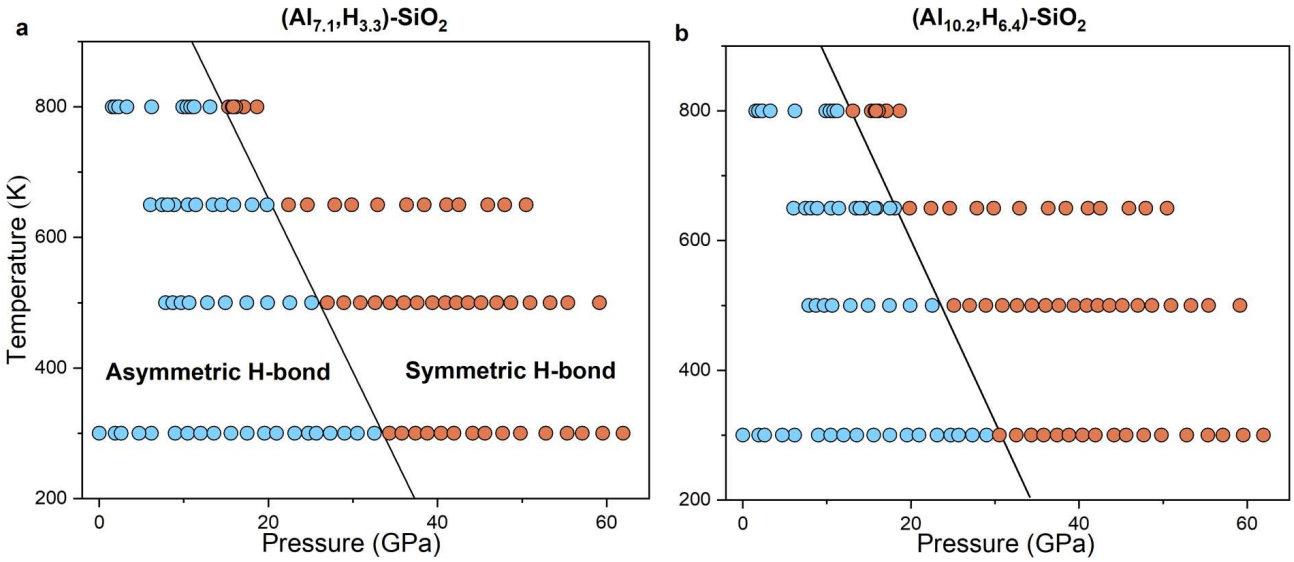


**Fig. 2| Phase diagram of hydrogen bond symmetrization in (Al,H)-bearing $CaCl_2$-type $SiO_2$ at high pressures and temperatures.**