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SMP045-03 会場:301B 時間:5 月 24 日 14:45-15:00

歪んだルチル型の含水鉱物における大きな D/H 同位体効果
D/H itosope effects in distorted rutile type hydrous minerals

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delta-AlOOH, distorted rutile type oxyhydroxide is an important hydrous mineral in the deep earth that is stable at the lower mantle condition. Theoretical studies have pointed out that hydrogen would locate at the center between two oxygen atoms at high pressure, which is so called symmetrization of the hydrogen bond. X-ray diffraction study found the difference in the pressure where compression behavior change, suggests there is D/H isotope effect. To investigate D/H isotope effect in the pressure response of strong hydrogen bond in delta-AlOOH, Neutron diffraction experiment is conducted at SNAP in SNS, Oak Ridge.

High pressure was obtained using a Paris-Edinburgh high-pressure cell with BN anvils. About 100 mg of powder sample was loaded into a null-scattering TiZr alloy encapsulating gasket. Deuterated methanol-ethanol was used as a pressure medium. The diffraction pattern was collected by the detector at the angle of 90 degrees. Pressure was calculated using an equation of state of delta-AlOOH determined by X-ray diffraction study. The structure was refined by means of Rietveld method using GSAS and EXPGUI software package. The data was collected at 0, 2.5, 4.1, 5.6, 6.7, 7.1 GPa.

The intensity of 120 reflection continues to decrease at high pressure and become almost zero intensity at 6.7 GPa, suggesting the transition from P21nm to Pnnm as a precursor of symmetrization. This pressure condition is slightly lower than the pressure where the change in compressibility was observed. Strong D/H isotope effect was found in hydrogen bond geometry; O-H distances are longer than O-D, and H...O distances are shorter than D...O at the same pressure condition, whereas O...O distances do not show significant discrepancies. Present result is consistent with the previous study that found the change in compressibility of delta-AlOOH at high pressure than deuterated delta-AlOOD.