

Investigation of H-D isotope effect in a hydrous mineral using neutron diffraction

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The isotope fractionation factor is important to discuss the origin of minerals and rocks because it is affected by the environment of where the mineral is formed. Hydrogen and deuterium is known to have a large isotope fractionation that comes from a difference in mass. Based on experiments at ambient pressure, Graham et al (1980) indicated the importance of O-H...O geometry on D/H isotope fractionation showing that the mineral with shorter O...O distance of hydrogen bond tends to deplete in deuterium. This result suggests the importance of pressure effect on hydrogen isotope fractionation because the pressure changes the O...O distance in minerals significantly.

In this study, we investigated the evolution of hydrogen bond geometry in distorted rutile type mineral gyanite (CrOOH) under pressure using neutron diffraction. This mineral is known to have a large difference in the unit cell volume between CrOOH and CrOOD at ambient pressure. However the previous X-ray diffraction study (Sano-Furukawa et al., 2012) has indicated that this volume difference merges at around 5 GPa. We attempt to explain the cause of the phenomena from the crystallographic view.

Neutron diffraction experiment was conducted at the PLANET beamline in J-PARC by using Paris-Edinburgh press. We observed the change in deuterium distribution from order to disorder at around 3~5 GPa. In the presentation, the relation between the change of hydrogen bond geometry and reduced partition function ratio will be discussed.

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