

Introduction of TOF neutron diffraction experiments at high pressure -Determination of hydrogen positions in hydrous minerals-

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Hydrogen is the most abundant element in the solar system. Most of hydrogen is fixed as H₂O near the surface of the earth. H₂O interacts with some minerals and forms a variety of hydrous minerals. Some hydrous minerals are brought into the earth's interior and their dehydration reactions at certain pressure-temperature conditions are closely related with the magma genesis. Some hydrous minerals are known to be stable in the mantle and should have significant effects on properties of the mantle.

Crystal structures of hydrous minerals provide fundamental information for better understanding of physical and chemical properties on their minerals. Since hydrogen has a small scattering cross section for X-rays, it is difficult to determine hydrogen positions in hydrous minerals. Although well-sophisticated X-ray diffraction techniques with synchrotron X-ray sources recently give opportunities of accurate determinations of hydrogen positions at ambient conditions, the collection of the good quality data at high pressure and/or high temperature is still challenging. On the other hand, it has been recognized that neutrons are powerful probe for determining hydrogen positions (cf. Hydrogen atoms are usually exchanged for deuterium atoms, because deuterium has a larger scattering cross section than does hydrogen.). Even *in situ* neutron diffraction studies at high pressures have provided several successful results. We have performed TOF neutron diffraction experiments for some hydrous minerals such as hydroxides, hydro-carbonates and hydrous silicates at the beamlines in ISIS, UK. Now new generation spallation neutron facilities are under construction in Tokai, Japan and our beamline designed for TOF measurements at high pressure and temperature is waiting for the budget.

We will talk about some our experiences of TOF neutron diffraction experiments in order to discuss the possibility and limitation of TOF neutron experiments at high pressure and high temperature. Our studies mainly determined hydrogen positions in some hydrous minerals at high pressures to see what happens in hydrogen bonding with increasing pressure.