

Hydrogen site analysis of hydrous ringwoodite in mantle transition zone by pulsed neutron diffraction

N. PUREVJAV^{1*}, T. OKUCHI¹ AND N. TOMIOKA^{1°}

¹Institute for Study of the Earth's Interior, Okayama University, (827 Yamada, Misasa, 682-0193, Tottori, Japan) (*narangoo@s.okayama-u.ac.jp; okuchi@misasa.okayama-u.ac.jp)

[°]Present address: Kochi Institute for Core Sample Research, Japan Agency for Marine-Earth Science and Technology (Nankoku, 783-8502, Kochi, Japan; tomioka@jamstec.go.jp)

Water is continuously transported into the deep mantle by subducting oceanic plates, while it partly reaches the mantle transition zone at depths between 410 km and 660 km. Here, wadsleyite and ringwoodite are the dominant constituents, which are high-pressure polymorphs of olivine [(Mg,Fe)₂SiO₄]. Wadsleyite and ringwoodite can incorporate up to 3 wt.% of water within their crystal structures. The hydrogen incorporates to exchange with Mg²⁺, Fe²⁺ or Si⁴⁺ in their structures. This exchanging mechanism significantly affects on physical properties of wadsleyite and ringwoodite such as seismic wave velocities and electrical conductivities. In order to interpret the geophysical observations of the transition zone it is essential to understand the hydration mechanism of them.

In this study, we aimed to elucidate the atomistic hydration mechanism of ringwoodite using pulsed neutron diffraction. Deuterated ringwoodite was synthesized by using the Kawai-type cell. Starting materials were San Carlos olivine [(Mg_{0.91}Fe_{0.09})₂SiO₄] powder and D₂O water. These reagents were sealed into the Au capsule, which was compressed to 19 GPa and then heated at 1300°C for 5 min. Up to 45 mg of homogenous powder of deuterated ringwoodite was successfully synthesized by each single run. The run products were identified to be ringwoodite with refined lattice parameter by X-ray diffractometry. Deuteration of the ringwoodite was revealed by Raman spectroscopy measurements. Deuterated ringwoodite of 66 mg was prepared from the two run products and used for neutron diffraction at BL-19 (TAKUMI) at the J-PARC. The neutron diffraction pattern was analyzed by using the Z-Rietveld code [1] to determine the position and site occupancies of deuterium atom in the ringwoodite structure. It was demonstrated that deuterium exchanges with both Mg²⁺, Fe²⁺ (M site) and Si⁴⁺ (T site) simultaneously [2].

[1] Oishi et al., (2009), Nucl. Instrum. Meth. A, 600(1), 94–96.

[2] Purevjav et al., (2014) Geophys. Res. Lett., 41, 6718–6724.