Neutron diffraction study of phase G

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We carried out a neutron powder diffraction study to determine the sites occupied by hydrogen in the structure of DHMS phase G, which is a candidate of a water reservoir in the transition zone and lower mantle. The diffraction data from deuterated sample (about 2.4 mg) were collected by using a highly sensitive imaging plate detector at the BIX-3 beamline at JRR-3M nuclear plant in JAERI Tokai Laboratory, Japan.

A powder of deuterated phase G was synthesized from a mixture of MgO, SiO2 and Mg(OD)2, which was prepared by heating MgO and D2O in a silica glass tube at 200 C for two months. The synthesis conditions of the deuterated sample was 1273K and 20 GPa.

The Rietveld method was applied to refine the structure, using the refinement program RIETAN-94. The present neutron diffraction data reveal that deuterium is located in the 6k site of Wykoff letter in the MO6 layer of the phase G structure with the space group P-31m. The bond length of O-D bond is 0.8(3) angstrom.