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High P-T neutron diffraction studies of hydrous minerals

Y. Zhao, H. Xu, D.D. Hickmott, J. Zhang, L.L. Daemen and S.C. Vogel LANSCE and EES Divisions, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Significant amounts of water are carried into the mantle at subduction zones in hydrous minerals formed in oceanic crust. Thus studying the stability of hydrous minerals at high pressure and high temperature conditions is important in determining the state of water in the Earth's interior and its effects on mantle rheology and melting. Since neutrons are more sensitive to hydrogen (and its isotope deuterium) than X-rays, in situ high-P/T neutron scattering is a powerful technique for such studies. Using the high-P/T toroidal anvil apparatus coupled with time-flight neutron diffraction at LANSCE, we have investigated the structural and dehydroxylation behavior of several hydrous minerals, including brucite, portlandite and jarosite. Rietveld analysis of the data allowed determination of not only unit-cell parameters but also atomic positions and atomic displacement parameters at various P/T conditions. The bulk moduli and dehydroxylation P/T conditions of these compounds have also been determined. These studies thus provide important insights into the mechanisms of water storage and transport in the deep Earth.