American Crystallographic Association 2010 Annual Meeting: Abstract 0281
Chicago, IL July 24-29 2010

Single-crystal neutron diffraction study of hydrous wadsleyite: hydrogen positions for H_2O incorporation into Earth's deep interior

Steven D. Jacobsen[1], Joseph R. Smyth[2], Matthias Gutmann[3], Daniel J. Frost[4], Erik Hauri[5], and Craig R. Bina[1]

[1]Department of Earth and Planetary Sciences, Northwestern University, USA
[2]Department of Geological Sciences, University of Colorado, USA
[3]Rutherford Appleton Laboratory, ISIS Facility, Chilton Didcot, United Kingdom
[4]Bayerisches Geoinstitut, University of Bayreuth, Germany
[5]Department of Terrestrial Magnetism, Carnegie Institution of Washington, USA

Wadsleyite (β-Mg_2SiO_4) is a nominally anhydrous, high-pressure polymorph of olivine and considered one of the major mantle phases at 410-520 km depth. Wadsleyite (orthorhombmic, *Imma*) has a remarkable ability to include H at very high pressures and temperatures through hydroxyl defects associated with O1, an underbonded oxygen site that is coordinated to five octahedral-Mg sites and not to Si (e.g. Smyth 1987). At conditions of the upper mantle, wadsleyite can incorporate up to several weight percent of H_2O into its structure, making it potentially one of the largest H_2O reservoirs in the global water cycle. X-ray crystallographic studies of H in wadsleyite have inferred proton positions from *R*(O…O) interatomic distances in conjunction with polarized infrared spectroscopy, however no direct refinement of hydrogen positions in wadsleyite has been possible because of limited hydrogen concentrations (2 wt% H_2O in wadsleyite represents only about 2 H atoms per unit cell) and limited crystal sizes from high pressure synthesis above 12 GPa and 1200C. We report synthesis of a hydrous wadsleyite crystal about one mm in size using the large-volume, 5000 tonne multi-anvil press at Bayerisches Geoinstitut in Bayreuth, Germany. The sample contains 1.77 wt% H_2O, as measured by secondary ion mass spectrometery. The structure was investigated on the single-crystal diffraction (SXD) beamline of the ISIS pulsed-spallation neutron source at Rutherford Appleton Laboratory, UK. We integrated over 3000 time-of-flight reflections from three 24-hour exposures and carried out GSAS and Maximum Entropy Method refinements of the structure. Two hydrogen positions in the structure have been refined from the data. Methods and hydrogen-bonding environments in wadsleyite will be presented in detail.