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Compressibility of K(x)Na(1-x)MgF3 Endmember, KMgF3

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Beamline(s): X7A

Introduction: The perovskite structure is of the form ABX3. It consists of corner-sharing B-X octahedra that house A cations in 12-fold coordination. Interest in this unique structure stems from a central role in Earth Science: Ferroelastic phase transition(s) in the perovskite MgSiO3 may explain observed seismic discontinuities in Earth's lower mantle [Shim and Jeanloz 2002]. K(x)Na(1-x)MgF3 end member, NaMgF3, is isostructural to MgSiO3 and thus, may be used as a proxy for determining structural behavior at extreme conditions [O'Keeffe 1979]. Multiple industrial applications add interest to perovskite-structured materials, which have found applications ranging from substrates for superconductors [Kawasaki 1999] to electrolytes in solid state fuel cells [Ishihara 1996].

Methods and Materials: The polycrystalline sample of KMgF3 was prepared in air using conventional solid-state methods. High-resolution x-ray powder diffraction patterns were collected at a wavelength of .694133 angstroms using a position-sensitive detector with a spatial resolution of less than 50 microns. The 200 micron beam was obtained using a using a Si 220 focuing monochromator. A 16:4:1 methanol + ethanol + water solution was used as a pressure transmitting medium and pressure was calibrated using the ruby fluorescence scale.

Results: Nine diffraction patterns were collected up to 8.74 GPa. Rietveld analysis indicates perovskite KMgF3 remains cubic in space group Pm-3m throughout all pressures reached in this experiment. Bulk modulus was obtained by plotting normalized pressure (F) vs. strain (f) see Hienz and Jeanloz (1984). A preliminary value of bulk modulus is estimated at 86 GPa by fitting a straight line to data points on the F vs, f plot.

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