Compressibility and Structural Evolution of Post-perovskite Phase under Pressure

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The post-perovskite (ppv) phase of $(Mg,Fe)SiO_3$ is of major significance for understanding the D" layer at the base of Earth's mantle. Here we report equation of state (EoS) and Rietveld refinement data of MgGeO3-ppv phase (CaIrO3-type, Cmcm) together with EoS data of silicate-ppv phase experimentally determined for the first time.

Germanate and silicate ppv phases were synthesized from MgGeO3 and Mg0.9Fe0.1SiO3 orthopyroxene at 86 GPa, ~1600 K and 103 GPa, ~1900 K, respectively, using laser-heated diamond cells with Ar or NaCl pressure medium. Angle-dispersive X-ray diffraction experiments were conducted at 13-ID-D, Advanced Photon Source. EoS data (bulk modulus, its pressure derivative, and room pressure unit cell volume) were obtained using Birch-Murnaghan EoS to be 203(6) GPa, 4.4, 179.7(9) A^3 for MgGeO3-ppv and 219(5) GPa, 4.4, 164.9(6) A^3 for silicate-ppv. Rietveld refinement of MgGeO3-ppv was performed using GSAS/EXPGUI. A change in compression mechanism was found at ~45 GPa. Although b-axis is the most compressible axis in the pressure range investigated, it is significantly more compressible at the lower pressure range. The reason is explained by decrease of distortion of GeO6 octahedron in the lower pressure range, and by both increase of distortion of GeO6 octahedron and shortening of Mg-O distances in the higher pressure range.

Keywords: high-pressure phases, x-ray powder diffraction, rietveld refinement