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Rietveld structure refinement of $MgGeO_3$ post-perovskite phase to 1 Mbar

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Abstract

Using the $CaIrO_3$-type structure model (space group *Cmcm*), lattice parameters and atomic positions of the $MgGeO_3$ post-perovskite (pPv) phase were determined based on Rietveld refinements at 78–109 GPa and first-principles calculations based on density functional theory. The reproducibility of structural parameters obtained for different samples, consistency with theoretical calculations, and good agreement with expected bond lengths based on structurally similar materials all provide evidence for both validity of $CaIrO_3$-type structure model for the pPv phase in $MgGeO_3$ exceeding 1 Mbar and reliability of structural parameters obtained by Rietveld refinements approaching 1 Mbar. The $MgGeO_3$ pPv phase exhibits strong anisotropy in axial compressibility, with the **b**-axis being most compressible. The polyhedral bulk modulus for the GeO_6 octahedron is 1.9× larger than that for the MgO_8 hendecahedron. Examination of neighboring O-O distances shows that the O-O distance aligned along the **a** direction is one of the longest and that aligned along **c** is one of the shortest, and these may be related to the lower compressibility along **c** compared with **a**. Comparison of structural features of $MgGeO_3$ pPv with those for $MgSiO_3$, $NaMgF_3$, and $CaIrO_3$ pPv show that $MgSiO_3$ pPv has more similarity with $NaMgF_3$ and $MgGeO_3$ pPv than with $CaIrO_3$ pPv in such parameters as degree of octahedral distortion, implying that both $NaMgF_3$ and $MgGeO_3$ pPv are better analogs to $MgSiO_3$ pPv than $CaIrO_3$ pPv.

Keywords: Post-perovskite, $MgGeO_3$, Rietveld refinement, high-pressure experiment, first-principles calculation, laser-heated diamond anvil cell, density functional theory, polycrystalline X-ray diffraction