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Equation of state and hyperfine parameters of high-spin bridgmanite in the Earth's lower mantle by synchrotron X-ray diffraction and Mössbauer spectroscopy

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ABSTRACT

In this study, we performed synchrotron X-ray diffraction (XRD) and Mössbauer spectroscopy (SMS) measurements on two single-crystal bridgmanite samples [$Mg_{0.94}Fe^{2+}_{0.04}Fe^{3+}_{0.02}Al_{0.01}Si_{0.99}O_3$ (Bm6) and $Mg_{0.89}Fe^{2+}_{0.024}Fe^{3+}_{0.096}Al_{0.11}Si_{0.89}O_3$ (Al-Bm11)] to investigate the combined effect of Fe and Al on the hyperfine parameters, lattice parameters, and equation of state (EoS) of bridgmanite up to 130 GPa. Our SMS results show that Fe^{2+} and Fe^{3+} in Bm6 and Al-Bm11 are predominantly located in the large pseudo-dodecahedral sites (A-site) at lower-mantle pressures. The observed drastic increase in the hyperfine quadrupole splitting (QS) between 13 and 32 GPa can be associated with an enhanced local distortion of the A-site Fe^{2+} in Bm6. In contrast to Bm6, the enhanced lattice distortion and the presence of extremely high QS values of Fe^{2+} are not observed in Al-Bm11 at high pressures. Our results here support the notion that the occurrence of the extremely high QS component of approximately 4 mm/s in bridgmanite is due to the lattice distortion in the high-spin (HS) A-site Fe^{2+}, instead of the occurrence of the intermediate-spin state. Both A-site Fe^{2+} and Fe^{3+} in Bm6 and Al-Bm11 remain in the HS state at lower-mantle pressures. Together with XRD results, we present the first experimental evidence that the enhanced lattice distortion of A-site Fe^{2+} does not cause any detectable variation in the EoS parameters, but is associated with anomalous variations in the bond length, tilting angle, and shear strain in the octahedra of Bm6. Analysis of the obtained EoS parameters of bridgmanite at lower-mantle pressures indicates that the substitution of Fe in bridgmanite will cause an enhanced density and a reduced bulk sound velocity (V_Φ), whereas the Al and Fe substitution has a reduced effect on density and a negligible effect on V_Φ. These experimental results provide new insight into the correlation between lattice, hyperfine, and EoS parameters of bridgmanite in the Earth's lower mantle.

Keywords: Bridgmanite, lattice distortion, equation of state, Fe and Al, lower mantle, high spin