

Single-crystal X-ray diffraction on the structure of (Al,Fe)-bearing bridgmanite in the lower mantle

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ABSTRACT

Here we have performed single-crystal X-ray diffraction (SCXRD) experiments on two high-quality crystal platelets of (Al,Fe)-bearing bridgmanite ($\text{Mg}_{0.88}\text{Fe}_{0.065}^{3+}\text{Fe}_{0.035}^{2+}\text{Al}_{0.03}(\text{Al}_{0.11}\text{Si}_{0.90})\text{O}_3$ (Fe10-Al14-Bgm) up to 64.6(6) GPa at room temperature in a Boehler-Almax type diamond-anvil cell. Refinements on the collected SCXRD patterns reveal reliable structural information of single-crystal Fe10-Al14-Bgm, including unit-cell parameters, atomic coordinates, and anisotropic displacement parameters. Together with Mössbauer and electron microprobe analyses, our best single-crystal refinement model indicates that the sample contains ~6.5 mol% Fe^{3+} , 3.5 mol% Fe^{2+} , and 3 mol% Al^{3+} in the large pseudo-dodecahedral site (A site), and ~11 mol% Al^{3+} in the small octahedral site (B site). This may indicate that Al^{3+} in bridgmanite preferentially occupies the B site. Our results show that the compression of Fe10-Al14-Bgm with pressure causes monotonical decreases in the volumes of AO_{12} pseudo-dodecahedron and BO_6 octahedron (V_A and V_B , respectively) as well as the associated A-O and B-O bond lengths. The interatomic angles of B-O1-B and B-O2-B decrease from 145.2–145.8° at 4.2(1) GPa to 143.3–143.5° at 64.6(6) GPa. Quantitative calculations of octahedral tilting angles (Φ) show that Φ increases smoothly with pressure. We found a linear relationship between the polyhedral volume ratio and the Φ in the bridgmanite with different compositions: $V_A/V_B = -0.049\Phi + 5.549$. Our results indicate an increased distortion of the Fe10-Al14-Bgm structure with pressure, which might be related to the distortion of A-site Fe^{2+} . The local environmental changes of A-site Fe^{2+} in bridgmanite could explain previous results on the hyperfine parameters, abnormal lattice thermal conductivity, mean force constant of iron bonds and other physical properties, which in turn provide insights into our understanding on the geophysics and geochemistry of the planet.

Keywords: (Al,Fe)-bearing bridgmanite, crystal structure, single-crystal X-ray diffraction, lower mantle, site distortion