Effects of ferric iron on observable properties of the lower mantle

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Heterogeneity in abundance of iron, Earth's densest major element, has been suggested to play an important role in mantle dynamics. However, quantifying iron-content in the deep mantle based on geophysical observations has been difficult, due in part to the complexity of incorporation of iron in multiple major minerals, crystallographic sites, and electronic valence and spin states. Few studies of the lower mantle's dominant mineral, $(Mg,Fe,Al)(Fe,Al,Si)O_3$ bridgmanite, have clearly distinguished the effects of Fe^{2+} and Fe^{3+} on observable physical properties. In addition, electronic spin transitions have been predicted to occur in bridgmanite by density functional theory (DFT), but experimental observations have been interpreted to demonstrate a wide variety of measured spin transition pressures and pressure ranges. To resolve controversy on the effects of high- and low-spin ferric iron on physical properties of bridgmanite, we examined a well-characterized $(Mg_{0.46}Fe^{3+}_{0.53})(Si_{0.49}Fe^{3+}_{0.51})O_3$ bridgmanite at pressures up to 85 GPa in the diamond anvil cell by synchrotron X-ray diffraction, X-ray emission spectroscopy, nuclear forward scattering, and 4-probe electrical resistivity. The results demonstrate that the spin transition in Fe^{3+} in the bridgmanite octahedral site is centered at 48-49 GPa at 300 K, in excellent agreement with DFT. The change in volume associated with the spin transition is ~1.9%, consistent with the lowest predicted values for the magnitude of this effect. Electrical conductivity of Fe^{3+}-bearing bridgmanite increases monotonically with pressure, with a slight change in slope within the pressure range of the transition. These effects are more subtle than observations in some previous studies and can be easily reconciled with observations of smooth variation of density and electrical conductivity in the mantle, especially at mantle-relevant temperatures. Above the spin transition pressure, densities of Fe^{3+}-bearing and Fe^{2+}-bearing bridgmanite are indistinguishable.