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Single-crystal equations of state of magnesiowüstite at high pressures

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Abstract

Solid solutions of (Mg,Fe)O with high iron enrichment may be an important component of ultralow-velocity zones at Earth's core-mantle boundary. However, to date there have been few high-precision studies on the elastic properties of these materials. In this study we present results on the compression of $(Mg_{0.22}Fe_{0.78})O$ magnesiowüstite in both neon and helium pressure media using single-crystal diffraction to ~55 GPa. In addition, our sample was characterized by time-domain synchrotron Mössbauer spectroscopy at ambient pressure using an extended time range that resulted in vastly improved energy resolution. The combination of these high-resolution techniques tightly constrains the presence of a defect-structure component at room pressure due to 4.7 mol% tetrahedrally coordinated ferric iron, resulting in a renormalized composition of $(Mg_{0.215}Fe_{0.762}\square_{0.023})O$. Both high-pressure diffraction data sets are well described by a third-order Birch-Murnaghan equation of state. The best fit-parameters for a crystal with cubic structure in helium are K_{0T} = 148(3) GPa, K'_{0T} = 4.09(12), and V_0 = 78.87(6) Å^3. Increasing differential stress in the neon-containing sample chamber was correlated with increasing apparent distortion of the initially cubic unit cell, requiring a lower-symmetry hexagonal cell to fit the data above ~20 GPa. For fit equations of state, we determine the pressure-dependent correlation ellipses for the equation of state parameters and compare with previously published single-crystal diffraction data from (Mg,Fe)O crystals in a helium medium. We make two main observations from the data sets using a helium pressure medium: K_{0T} decreases as a function of increasing iron content from periclase to wüstite and K'_{0T} is consistent with an approximately constant value of 4.0 that is independent of iron content, at least up to the iron concentration measured here. In combination with previously reported thermal parameters, we compute the density of magnesiowüstite with this composition at core-mantle boundary conditions and discuss the implications.

Keywords: Magnesiowüstite, single-crystal diffraction, elasticity, equations of state, Mössbauer spectroscopy, high pressure