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 (Mg0.22Fe0.78)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 (Mg0.215Fe0.7620.023)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′0 = 148(3) GPa, K″0 = 4.09(12), and V0 = 78.87(6) Å3. 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′0 decreases as a function of increasing iron content from periclase to wüstite and K″0 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

INTRODUCTION

Ferromagnesian oxides are a primary component of the Earth’s lower mantle, along with the dominant bridgmanite and minor CaSiO3 perovskite phases (Irifune 1994; Tschauner et al. 2014). While the bulk of the lower mantle likely contains (Mg,Fe)O ferropericlase solid solutions with ~10–40 mol% of FeO (Fei et al. 1996; Mao 1997; Simmyo et al. 2008), the presence of material significantly more enriched in Fe has been hypothesized as an explanation for some of the complex seismic structure observed near the core-mantle boundary (CMB). In particular, ultralow-velocity zones (ULVZs), tens of kilometer-thick patches at the CMB, show a ~10% reduction in seismic P-wave velocity and a ~30% reduction in seismic S-wave velocity from average lower-mantle values (Wen 1998; Thorne and Garnero 2004; Rost et al. 2006).

While several suggestions have been put forth in the literature to explain the origin of these features (Manga and Jeanloz 1996; Williams et al. 1998; Mao et al. 2006), one hypothesis that has gained traction in recent years proposes Fe-rich oxide components to explain the observed low sound velocities. Work by Wicks et al. (2010) used nuclear resonant inelastic scattering to show that the shear velocity of (Mg0.16Fe0.84)O magnesiowüstite was ~55% slower than end-member MgO at CMB pressures, and that only ~10 vol% of this material mixed with a silicate assemblage would be needed to match ULVZ seismic velocities. Subsequent simulations (Bower et al. 2011) that explored the geodynamic effects of enriching ULVZ material with magnesiowüstite produced morphologies consistent with observed ULVZ seismic topography (Sun et al. 2013).

While selected properties of (Mg,Fe)O with low iron concentrations have been determined at pressures above 1 Mbar and temperatures over 2000 K (Westrenen et al. 2005; Lin et al. 2006, 2007; Mao et al. 2011), until recently, the iron-rich members of this solid solution received less attention (Ohta et al. 2014;