Static compression of \((\text{Mg}_{0.83}\text{Fe}_{0.17})\)O and \((\text{Mg}_{0.75}\text{Fe}_{0.25})\)O ferropericlase up to 58 GPa at 300, 700, and 1100 K

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ABSTRACT

Static compression data of \((\text{Mg}_{0.83}\text{Fe}_{0.17})\)O and \((\text{Mg}_{0.75}\text{Fe}_{0.25})\)O ferropericlases have been measured up to 58 GPa along 300, 700, and 1100 K isotherms, using synchrotron powder X-ray diffraction experiments combined with a Kawai-type, multi-anvil, high-pressure apparatus and sintered diamond anvils. High-temperature and high-pressure equations of state for these two ferropericlases, which have high-spin \(\text{Fe}^{2+}\) ions, were developed using measured compression data below 47 GPa, based on the Mie-Grüneisen relation and the Debye thermal model, combined with the 300 K Birch-Murnaghan equation. When the isothermal bulk modulus \(K_0\) and the Debye temperature \(\Theta_0\) are fixed at 160 GPa and 500 K, respectively, the optimized equation-of-state parameters for these two phases are as follows: the pressure derivative of the bulk modulus \(K_0\), the Grüneisen constant \(\gamma\), and the q parameter are 4.08 ± 0.02, 1.53 ± 0.04, and 0.7 ± 0.2, respectively, for \((\text{Mg}_{0.83}\text{Fe}_{0.17})\)O; and 4.22 ± 0.03, 1.64 ± 0.04, and 0.7 ± 0.2, respectively, for \((\text{Mg}_{0.75}\text{Fe}_{0.25})\)O. We found that calculated pressures with these equation-of-state parameters accurately reproduce the measured pressures of each ferropericlase below ~50 GPa for the isotherms of 300, 700, and 1100 K. Furthermore, the compression curve indicates that for each ferropericlase at each isothermal compression of 300, 700, and 1100 K, an abrupt volume reduction occurs at ~50 GPa. This volume reduction becomes more pronounced with increasing pressure, as a result of the progressive transition from high-spin to low-spin of the \(\text{Fe}^{2+}\) ions in each ferropericlase.

Keywords: Static compression, ferropericlase, high pressure, spin transition, high temperature, lower mantle

INTRODUCTION

Ferropericlase \((\text{Mg,Fe})\)O (Fp), with FeO content of 10–20 mol%, is considered to be a main constituent of the Earth’s lower mantle, along with coexisting silicate perovskites \((\text{Mg,Fe,Al})\)SiO\(_3\) and CaSiO\(_3\) (e.g., Jeanloz and Thompson 1983; Ito and Takahashi 1989). It is of crucial importance to gain accurate knowledge of the elastic properties of Fp at high temperature and high pressure, and to investigate how its elasticity varies with FeO content, to understand the physical and chemical properties of the deep Earth. It is well known that Fe-rich \((\text{Mg,Fe})\)O solid solutions have considerable degrees of non-stoichiometry related to the presence of ferric iron \((\text{Fe}^{3+})\) and that deviation from stoichiometry generally increases with increasing FeO content (e.g., Jackson et al. 1978, 1990). However, Mg-rich stoichiometric Fp samples with \((\text{Mg} + \text{Fe})/\text{O} = 1\) demonstrate a fairly linear correlation between cubic cell parameter and FeO content (Jackson et al. 1978; Bonczar and Graham 1982; Jacobsen et al. 2002).

The measured bulk modulus of end-member periclase MgO at ambient conditions is constrained to have the adiabatic value \(K_{\text{OS}} = 162–163\) GPa and the isothermal value \(K_{\text{IT}} = 160\) GPa (Jackson and Niesler 1982; Sumino et al. 1983; Fei 1999); \(K_T\) is related to \(K_S\) by \(K_S = (1 + \alpha_T T) K_T\), where \(\alpha\) and \(T\) represent volume thermal expansivity, the Grüneisen parameter, and temperature, respectively. However, the FeO dependence of the bulk modulus in Fp is still under debate. Ultrasonic or Brillouin scattering measurements show that \(K_{\text{OS}}\) values remain nearly constant or increase slightly with FeO content for Fp containing less than ~40% FeO (Jacobsen et al. 2002; Kung et al. 2002; Jackson et al. 2006), as shown in Figure 1. However, according to static compression experiments (Zhang and Kostak 2002; van Westrenen et al. 2005; Fei et al. 2007b; Speziale et al. 2007; Komabayashi et al. 2010), \(K_{\text{OS}}\) value decreases slightly with FeO content, as seen in Figure 1. This discrepancy may be related in part to compositional difference arising from non-stoichiometry in Fp samples, the use of different pressure scales, the limited range of measured pressures, or different constraints on the equation of state (EOS) used in various static compression experiments.

The pressure-induced electronic transition of ferrous iron \((\text{Fe}^{2+})\) from high-spin (HS) to low-spin (LS) in Fp has been reported to begin at approximately 40–50 GPa at room temperature for samples containing 10–25 mol% FeO, based on Mössbauer and X-ray emission spectroscopy (Badro et al. 2003; Lin et al. 2005; Speziale et al. 2005). The two spin states coexist over an extended pressure range, which widens with increasing temperature, related to entropy effects (Tsuchiya et al. 2006;