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# Equation of state and spin crossover of (Mg,Fe)O at high pressure, with implications for explaining topographic relief at the core-mantle boundary

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## Abstract

Iron-bearing periclase is thought to represent a significant fraction of Earth's lower mantle. However, the concentration of iron in (Mg,Fe)O is not well constrained at all mantle depths. Therefore, understanding the effect of iron on the density and elastic properties of this phase plays a major role in interpreting seismically observed complexity in the deep Earth. Here we examine the high-pressure behavior of polycrystalline (Mg,Fe)O containing 48 mol% FeO, loaded hydrostatically with neon as a pressure medium. Using X-ray diffraction and synchrotron Mössbauer spectroscopy, we measure the equation of state to about 83 GPa and hyperfine parameters to 107 GPa at 300 K. A gradual volume drop corresponding to a high-spin (HS) to low-spin (LS) crossover is observed between ~45 and 83 GPa with a volume drop of 1.85% at 68.8(2.7) GPa, the calculated spin transition pressure. Using a newly formulated spin crossover equation of state, the resulting zero-pressure isothermal bulk modulus $K_{0T,HS}$ for the HS state is 160(2) GPa with a $K'_{0T,HS}$ of 4.12(14) and a $V_{0,HS}$ of 77.29(0) Å$^3$. For the LS state, the $K_{0T,LS}$ is 173(13) GPa with a $K'_{0T,LS}$ fixed to 4 and a $V_{0,LS}$ of 73.64(94) Å$^3$. To confirm that the observed volume drop is due to a spin crossover, the quadrupole splitting (QS) and isomer shift (IS) are determined as a function of pressure. At low pressures, the Mössbauer spectra are well explained with two $Fe^{2+}$-like sites. At pressure between 44 and 84, two additional $Fe^{2+}$-like sites with a QS of 0 are required, indicative of low-spin iron. Above 84 GPa, two low-spin $Fe^{2+}$-like sites with increasing weight fraction explain the data well, signifying the completion of the spin crossover. To systematically compare the effect of iron on the equation of state parameters for (Mg,Fe)O, a spin crossover equation of state was fitted to the pressure-volume data of previous measurements. Our results show that $K_{0,HS}$ is insensitive to iron concentration between 10 to 60 mol% FeO, while the spin transition pressure and width generally increases from about 50–80 and 2–25 GPa, respectively. A key implication is that iron-rich (Mg,Fe)O at the core-mantle boundary would likely contain a significant fraction of high-spin (less dense) iron, contributing a positive buoyancy to promote observable topographic relief in tomographic images of the lowermost mantle.

**Keywords:** (Mg,Fe)O, ferropericlase, spin crossover, equation of state, X-ray diffraction, synchrotron Mössbauer spectroscopy, lower mantle, ultralow-velocity zones