Phase Transitions in Transition Metal Monooxides: Interplay Between Structural, Magnetic, and Electronic Properties

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The iron monoxide $Fe_{1-x}O$ (wüstite) is an important member of the highly correlated transition metal monoxide group which includes NiO, CoO, and MnO, and is also an end-member component of the (Mg,Fe)O solid solution, the most abundant non-silicate oxide in the Earth. At ambient conditions wüstite exists in a cubic fcc-based rock-salt structure with a nonstoichiometric formula $Fe_{1-x}O$. At low temperatures a rhombohedral distortion of the cubic cell is known to occur as believed to be driven by antiferromagnetic ordering. A strong C_{44} elastic constant softening is also observed in the same temperature range. At high pressures the cubic-to-rhombohedral phase transformation occurs in FeO, and C_{44} mode softening also exists at high pressures. Elastic mode softening was assigned to a strong magneto-elastic coupling in FeO. We conducted combined high-pressure and low- and high-temperature X-ray and neutron diffraction, Mössbauer spectroscopy, and ultrasonic interferometry study of FeO, FeO-MgO solid solutions, and MnO. We revealed decoupling of magnetic ordering and structural distortion in nonstoichiometric FeO in a wide temperature (up to 1100 K) and pressure (over 100 GPa) range. For MnO we observed strong correlation between magnetic ordering and structural transition at ambient pressure and could not distinguish Neel (TN) and structural transition (TS) temperatures within experimental uncertainties. The pressure dependence of TN and TS in MnO, however, are different at elevated pressures, like in case of FeO. Cubic-to-rhombohedral phase transition was observed for ferropericlase Mg0.8Fe0.2O at about 40 GPa and no transformation was observed in Mg0.95Fe0.05O at pressures up to 80 GPa. The existence of a rhombohedral distortion in ferropericlase with mantle composition at high pressures coupled with the absence of magnetic ordering has important implications for the interpretation of seismological data with respect to Earth lower mantle inhomogeneity.

Keywords: high-pressure, magnesiowüstite, phase transitions