The Bulk Modulus Systematics for B1-Structured 3d Transition-Metal Monoxides: Prediction for the Bulk Modulus of Stoichiometric FeO *	X17B1

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The rock salt structured monoxides play an important role as model systems in understanding complexities in bonding characteristics, defect structure, and effect of nonstoichiometry on the physical properties. In view of the current ambiguity surrounding the effect of defect concentration on the bulk modulus of wustite [1] and a large spread of the bulk modulus values for NiO (K_0 = 173-220 GPa) ([2] and references therein), it seems that a systematic study of the elastic behavior of the 3d transition-metal monoxides might be fruitful.

NiO, CoO, and MnO have been studied under static pressure up to 8.3 GPa using energy-dispersive x-ray diffraction. NiO and CoO were studied in the single experiment so that the subtle difference in compressibility can be detected between these two compounds. The room-temperature volume data were collected exclusively after quench from 1073 K to minimize errors resulting from nonhydrostatic stress during room-temperature compression. The pressure-volume data are fitted to a Eulerian finite-strain equation of state, assuming a value of 4 for K_0. The bulk modulus values obtained from these analyses (209$\pm$3, 194$\pm$2, and 148$\pm$2 GPa, respectively for NiO, CoO, and MnO) are found to decrease linearly with ambient unit-cell volume. These results are consistent with predictions from crystal-field modeling in that the bulk modulus should increase through the sequence MnO, FeO, CoO, and NiO [2,3]. From the experimentally determined bulk modulus-volume systematics, the predicted bulk modulus for stoichiometric FeO is in the neighborhood of 175 GPa, which is in accord with the experimental determination for $Fe_{0.99}O$ [1]. The conclusion of a significant effect of nonstoichiometry on the elastic properties of Fe_xO [1] is thus indirectly confirmed by the internally consistent experimental results for other 3d transition-metal monoxides.

References:

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