Evidence for Effect of Nonstoichiometry on the Elastic Properties of Wustite *	X17B1

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The variation of elastic properties with defect concentration or stoichiometry, a fundamental problem in the study of defect materials, has generally not been well understood by either experiments or theories. The experimental constraints on this issue have, to date, mainly come from studies of wustite, an iron oxide that possesses rock-salt structure and exhibits a wide range of nonstoichiometry (0.88 $< x < 1$ in Fe_xO). The elastic moduli of these compounds have been extensively studied by dynamic and static measurements and found to be insensitive to degree of nonstoichiometry over a composition range x = 0.90 - 0.98 [1]. However, the bulk moduli of ideal stoichiometric FeO, predicted from crystal field contributions to the elastic moduli for the 3d transition-metal monoxides, are 15-20 percent larger than the experimentally determined values for Fe_xO [2,3]. This difference, inferring a possible effect of defect concentration on the elastic properties of wustite, has so far not been demonstrated by direct experimental evidence.

In this study, wustite (Fe_xO in the composition range x = 0.95-0.99) and MgO have been studied under static high pressure. The near stoichiometric wustite, $Fe_{0.99}O$, was obtained by exsolving magnetite (Fe_3O_4) from $Fe_{0.945}O$ via slow heating and cooling in the temperature range 300-1073 K at 1.93, 2.65 and 5.44 GPa, following a kinetically-controlled reaction $Fe_xO \rightarrow Fe_yO + Fe_3O_4$, with $y > x$ [15]. At ambient temperature, $Fe_{0.99}O$ is found to be less compressible than MgO and substantially less compressible than Fe_xO with $x < 0.98$. Such observations provide the only direct evidence of a significant effect of defect concentration on the elastic properties and support the results of crystal-field modeling for ideal stoichiometric wustite. The bulk moduli of Fe_xO show a discontinuous variation at compositions that are within predicted range for the defect clusters to form, a behavior that may be caused by an order-disorder transition of the defect structure.

References:

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* This work was supported by the NSF under a grant EAR 89-20239 to the Center for High Pressure Research, and by the DOE under contract number DE-AC02-98CH10886 to the NSLS.