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Possible polytypism in FeO at high pressures

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Abstract

Examination of X-ray diffraction intensities for FeO collected in situ at high pressure and high temperature reveals that the atomic arrangements of FeO in the hexagonal structure are not the same as those in the simple NiAs-type structure (B8) where Fe takes the place of Ni. The observed diffraction intensity can be explained by adding an anti-B8 component (where Fe takes the place of As). Substitution of Fe and O atoms for each other is crystallochemically unique. The exchange of Fe and O positions provides a critical measure of the change in chemical bonding. Our conclusion is consistent with the observed transition of FeO from an ionically bonded structure to a strongly covalent and metallic one. First-principles electronic structure computations using the linearized augmented plane wave (LAPW) method with the generalized gradient approximation (GGA) indicate that both B8 and anti-B8 should be antiferromagnetic, but only anti-B8 should be an insulator. The GGA and local density approximation (LDA) incorrectly compute anti-B8 as the ground state structure.