

Equation of state of magnetite and its high-pressure modification: Thermodynamics of the Fe-O system at high pressure

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ABSTRACT

Fe₃O₄ has been studied by high-pressure diffraction to 43 GPa. No major changes in the spinel-type structure of magnetite is observed below 21.8 GPa. At higher pressure a sluggish transition to a high-pressure modification, h-Fe₃O₄, is observed. The X-ray diffraction pattern of the high-pressure modification is consistent with the orthorhombic unit cell (CaMn₂O₄-type structure, space group *Pbcm*) recently proposed for h-Fe₃O₄ by Fei et al. (1999), however, it is also consistent with a more symmetric CaTi₂O₄-type structure (space group *Bbmm*). Bulk modulus values for magnetite, $K_{T0} = 217$ (2) GPa, and h-Fe₃O₄, $K_{T0} = 202$ (7) GPa, are calculated from the pressure-volume data using a third-order Birch-Murnaghan equation of state. A thermodynamic analysis of the Fe-O system at high pressure is presented. The proposed equation of state of h-Fe₃O₄ gives an increased stability of wüstite relatively to a two-phase mixture of iron and h-Fe₃O₄ compared to earlier equations of state and removes an inconsistency in the thermodynamic description of the Fe-O system at high pressure.