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

CAMILLA HAAVIK,[1] SVEIN STØLEN,[1,*] HELMER FJELLVÅG,[1] MICHAEL HANFLAND,[2] AND DANIEL HÄUSERMANN[2]

[1]Department of Chemistry, University of Oslo, Postbox 1033, N-0315 Oslo, Norway
[2]European Synchrotron Radiation Facility, B.P. 220, F-38043 Grenoble, France

ABSTRACT

Fe_3O_4 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-Fe_3O_4, is observed. The X-ray diffraction pattern of the high-pressure modification is consistent with the orthorhombic unit cell ($CaMn_2O_4$-type structure, space group *Pbcm*) recently proposed for h-Fe_3O_4 by Fei et al. (1999), however, it is also consistent with a more symmetric $CaTi_2O_4$-type structure (space group *Bbmm*). Bulk modulus values for magnetite, K_{70} = 217 (2) GPa, and h-Fe_3O_4, K_{70} = 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-Fe_3O_4 gives an increased stability of wüstite relatively to a two-phase mixture of iron and h-Fe_3O_4 compared to earlier equations of state and removes an inconsistency in the thermodynamic description of the Fe-O system at high pressure.