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Equation of state of the high-pressure Fe_3O_4 phase and a new structural transition at 70 GPa

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Abstract

We have investigated the high-pressure behavior of Fe_3O_4 by in situ X-ray diffraction measurements from 11 to 103 GPa. Up to 70 GPa, the previous observed high-pressure Fe_3O_4 phase (h-Fe_3O_4) is stable, with a $CaTi_2O_4$-type structure. The compression curve shows an abnormal volume contraction at about 50 GPa, likely associated with the magnetic moment collapse observed at that pressure. Fitting the compression data up to 45 GPa to the Birch-Murnaghan equation of state yields a bulk modulus, K_{T0} = 172 GPa, and V_0 = 277 Å^3, with fixed K' = 4. At a pressure between 64 and 73 GPa, a new structural transition was observed in Fe_3O_4, which can be attributed to a martensitic transformation as described by Yamanaka et al. (2008) for post-spinel structural transition. The diffraction data can be best fitted with a *Pnma* space group. No breakdown of Fe_3O_4 was observed up to at least 103 GPa. The new high-pressure polymorph is about 6% denser than the h-Fe_3O_4 phase at 75 GPa.

Keywords: h-Fe_3O_4, magnetite, high pressure, phase transition, post-spinel, XRD data