

High-pressure structural and magnetic behaviour of ϵ -Fe₂O₃ nanoparticles studied by powder X-ray diffraction and ⁵⁷Fe nuclear forward scattering

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ϵ -Fe₂O₃ is one of four crystalline polymorphs of ferric oxide [1]. It has remarkable magnetic properties [2] and recently published results indicate its probable multiferroic behaviour [3]. ϵ -Fe₂O₃ crystallizes in orthorhombic crystal system (space group $Pna2_1$). It has four independent atomic positions for iron and six for oxygen [4]. Three of the iron sites have octahedral coordination (Fe1, Fe2, and Fe3) and one has tetrahedral coordination (Fe4) (Figure 1). Each iron site gives rise to one magnetic sublattice, which form a ferrimagnetic arrangement of the magnetic moments at room temperature [4]. The polyhedra form chains along [100] and they are separated by channels.

Powder X-ray measurements (PXRD) were performed at P02 beamline and ⁵⁷Fe nuclear forward scattering (NFS) was measured at beamline P01. The data obtained were analysed using Fullprof program (XRPD) [5] and CONUSS program (NFS) [6]. The four magnetic sublattices were fitted with three spectral components due to very close hyperfine parameters of Fe1 and Fe2 components.

High pressure did not induce transformation of ϵ -Fe₂O₃ to hematite, but it induced unit cell compression. Lattice parameter a relatively increased up to approximately 2.5 GPa (Figure 2, left). The other ones monotonously decreased with increasing pressure. The anomalous behaviour of the lattice parameter a is in accord with the main feature of the structure: the chains of polyhedra running along [100] separated by channels.

The values of isomer and quadrupole shifts, and hyperfine fields of all spectral components did not show any abrupt change in the studied range of pressures. The hyperfine fields (Figure 2, right) showed a monotonous increase with pressure.

In conclusion, pressures up to 12 GPa do not induce any structural or magnetic changes in ϵ -Fe₂O₃ nanoparticles.

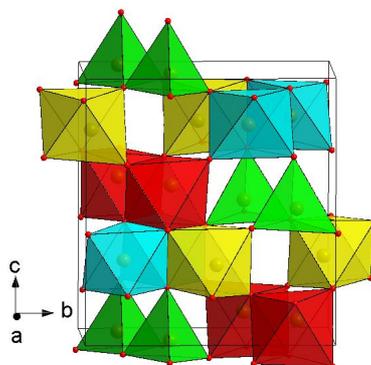


Figure 1: Structural model of ϵ -Fe₂O₃ at 200 K (Gich *et al.* 2006). Fe1, Fe2, Fe3 (octahedral), and Fe4 (tetrahedral) iron sites are labelled by red, yellow, blue, and green colours, respectively.

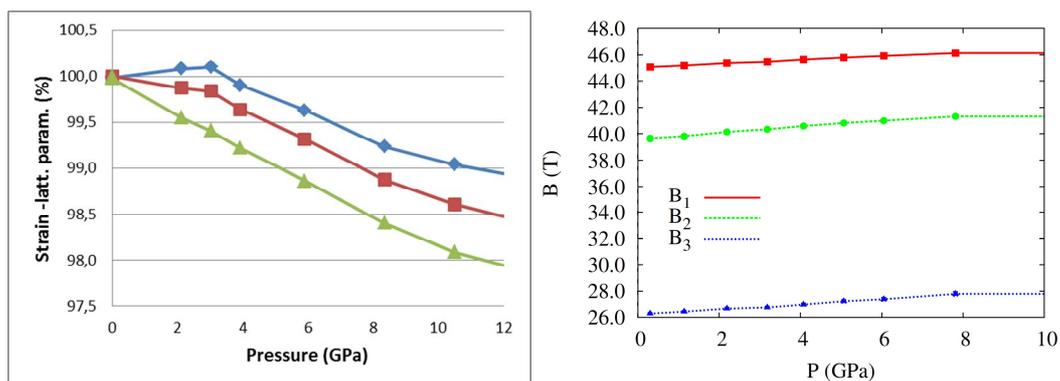


Figure 2: Left – dependence of strain of lattice parameters (a – blue, b – green, c – green) on applied pressure. Right – dependence of hyperfine field of Fe1+Fe2 (red), Fe3 (green), and Fe4 (blue) on applied pressure.

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References

- [1] L. Machala, J. Tuček, and R. Zbořil, Chem. Mater. **23**, 3255 (2011).
- [2] J. Jin, S. Ohkoshi, and K. Hashimoto Adv. Mater. **16**, 48 (2004).
- [3] Ch. Kadlec, F. Kadlec, V. Goian, M. Gich, M. Kempa, S. Rols, M. Savinov, J. Prokleška, M. Orlita, and S. Kamba Phys. Rev. B **88**, 104301 (2013).
- [4] M. Gich, J. Gazquez, A. Roig, A. Crespi, J. Fontcuberta, J.C. Idrobo, S.J. Pennycook, M. Varela, and V. Skumryev, Appl. Phys. Lett. **96**, 112508 (2010).
- [5] J. Rodriguez-Carvajal, Physica B **192**, 55 (1993).
- [6] W. Sturhahn, Hyperfine Interact. **125**, 149 (2000).