substance: Fe_3O_4
property: band structure

Only empirical energy level schemes are available [71B, 72C, 78T]. Quantitative calculations [73C, 75L, 79L] have been restricted to the one $t_{2g}\downarrow$ electron, an important feature of these calculations is that fractional charge density is permitted for $T < T_V$.

Empirical schemes from [72C] and [78T] are given in Fig. 1. Both predict O 2p – Fe 4s separations of ≈ 6...7 eV at RT. The main difference is in the relative position of the O 2p level to the Fe 3d orbitals. UPS-spectra (Figs. 2...4) clearly show that the initial absorption is due to the $t_{2g}\downarrow$ electron, then $e_g\uparrow$ B-site ionization before $t_{2g}\downarrow$ A-site ionization, in agreement with [78T]. High temperature transport data [81W] indicate a random distribution of mobile electrons over both A and B sites above 1450°C.

References:

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73C Cullen, J. R., Callen, E. R.: Phys. Rev. B7 (1973) 400.
75L Lorenz, B., Ihle, D.: Phys. Status. Solidi (b) 69 (1975) 451.
76A Alvarado, S. F., Erbudak, M., Munz, P.: Phys. Rev. B14 (1976) 2740.
78T Tossell, J. A.: Phys. Rev. B17 (1978) 484.
79L Lorenz, B., Ihle, D.: Phys. Status Solidi (b) 96 (1979) 659.
81W Wu, C., Mason, T. O.: J. Amer. Ceram. Soc. 64 (1981) 520.

Fig. 1.

Fe_3O_4. (a, b) Phenomenological band structures, (c) cluster calculation [72C, 78T] Δ_{ex}: exchange splitting of the d-orbitals, Δ_{cf}: crystal field splitted at the B sites, CL: cathodoluminescence onset fixing the Fe 3d, O 2p separation.

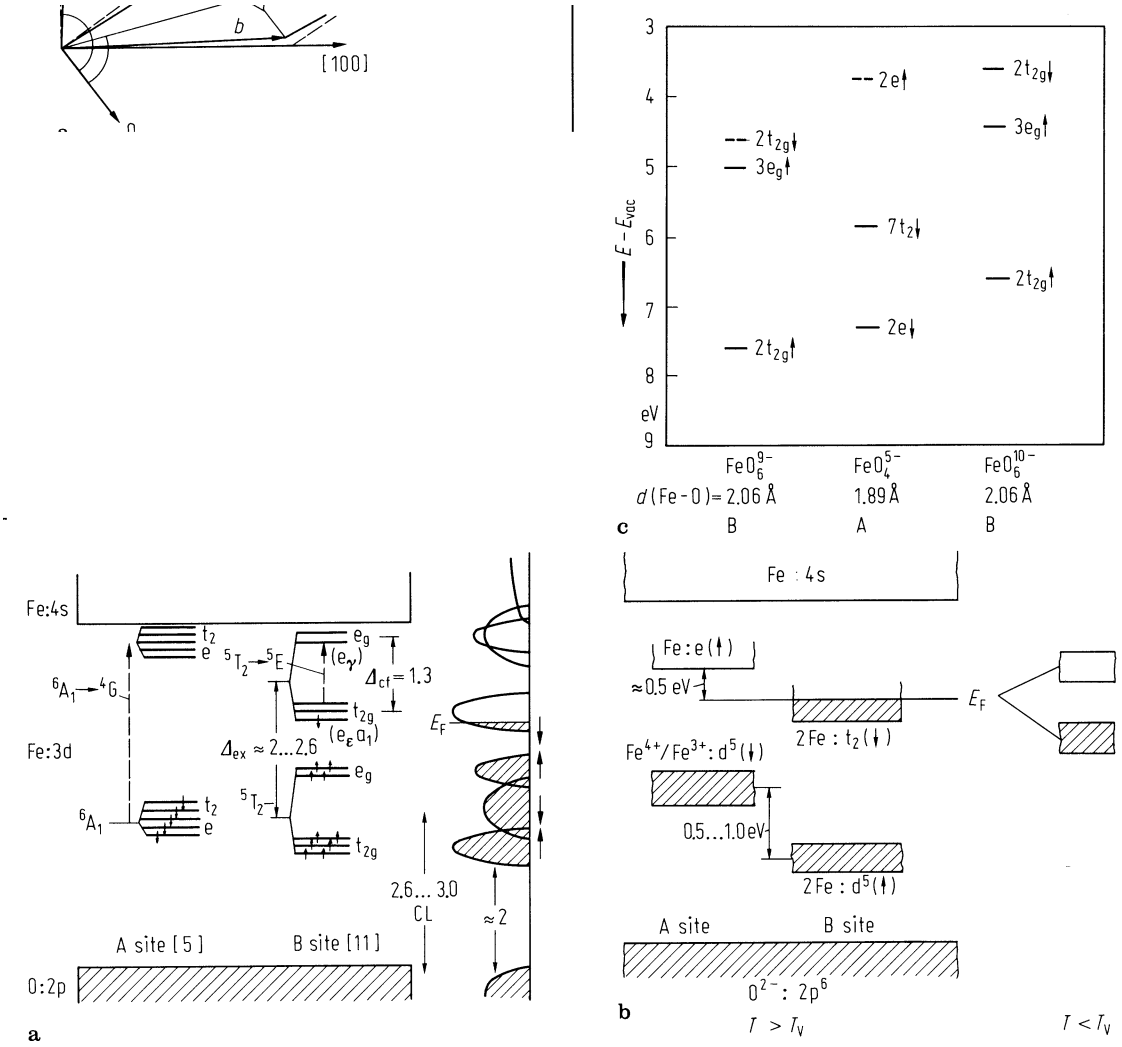

Fig. 2.

Fe_3O_4. Photoemission spectrum (intensity vs. electron binding energy) showing 3d emission as observed with synchrotron radiation (FUPS), with ultra-violet light (UPS) and as calculated with the single-ion-in-a-crystal-field (SICF) model [76A].

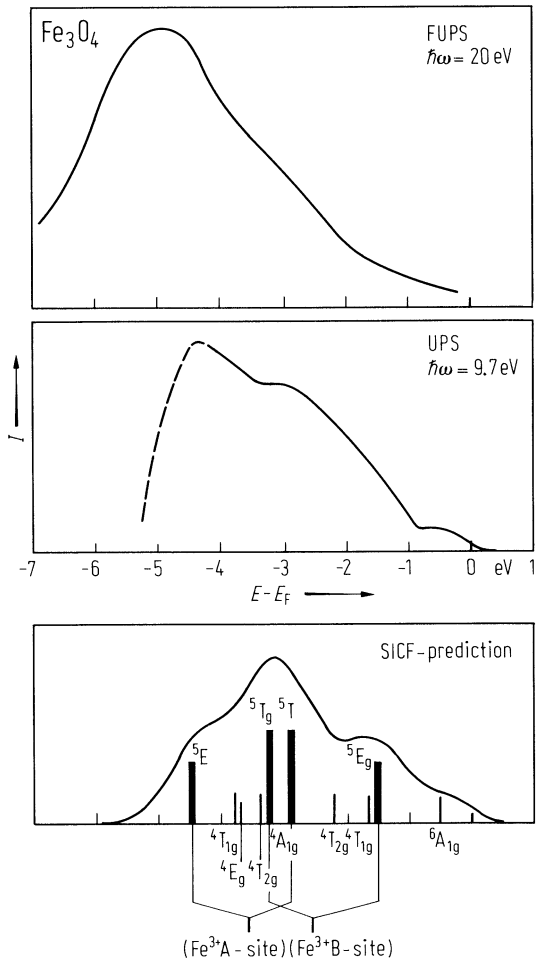

Fig. 3.

Fe_3O_4. Photoemission spectrum (intensity vs. electron binding energy) at two photon energies at 300 K. -·-·- inelastic background, ---- O 2p band, —— total energy distribution curves (EDC) and Fe 3d curve [76A].

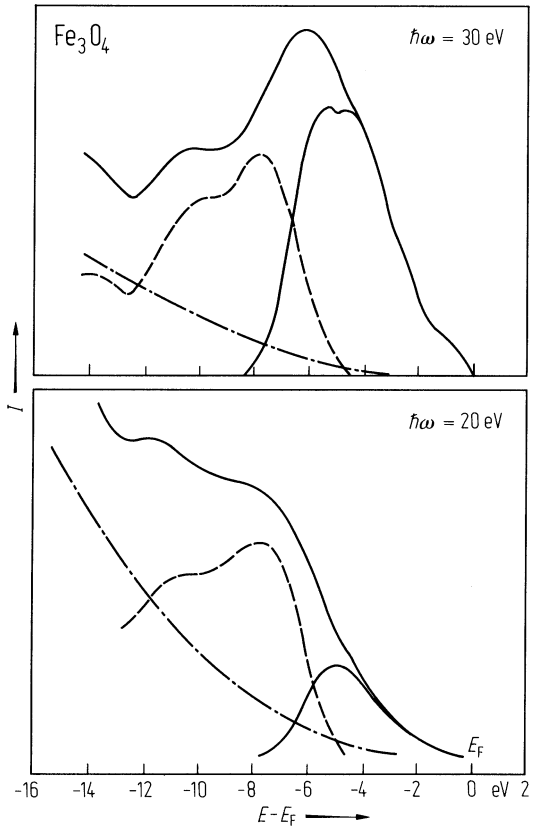

Fig. 4.

Fe_3O_4. Photoelectron spin polarization *P* vs. photon energy at 200 K. Lower curve: SICF prediction [76A].