substance: Co_3O_4
property: band structure energies

No band structure or cluster calculation appears to be available. XPE and UPE spectra have been reported (Figs. 1, 2). The assignment of the Co 3d region (Fig. 2) shows that very little energy apparently separates the Co^{2+} and Co^{3+} ionizations (ca. 0.5...1.0 eV). The O 2p band is ≈ 4 eV wide and is most clearly shown in the He II excitation (Fig. 1). Satellites in the core region have been explored for various Co-spinels, and tetrahedral Co^{2+} in $CoAl_2O_4$ and $CoCr_2O_4$ is characterized by Co 2p satellites at ca. 5...6 eV relative to the main $2p_{3/2,1/2}$ core levels whereas octahedral Co^{3+} is characterized by Co 2p satellites at ca. 9 eV [76O].
EELS peaks: 8.3(8) eV, 5 35.8(10) eV, 62.2(5) eV [77B].

References:

76O Oku, M., Hirokawa, K.: J. Electron Spectrosc. Relat. Phenom. 8 (1976) 475.
77B Balabanova, L. A., Stepin, E. V.: Fiz. Tverd. Tela 19 (1977) 3018.
79J Jugnet, Y., Duc, T. M.: J. Phys. Chem. Solids 40 (1979) 29.

Fig. 1.

Co_3O_4. Photoemission intensity vs. electron binding energy relative to Fermi energy for different photon energies showing valence band structure. *1*, *2* Co 3d ionization, *3*, *4* O 2p ionization, *5*, *6* ionization from and to states of Co 3d by configuration mixing [79J].

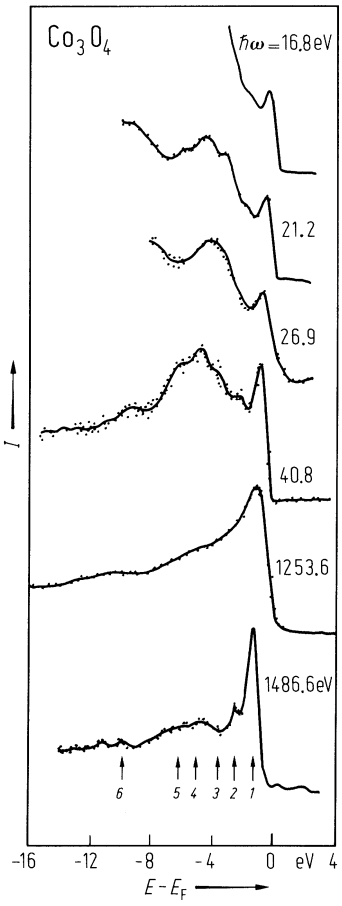

Fig. 2.

Co_3O_4. Detailed valence region PE spectra for He II and Al K_α exciting radiation: curves *d* and *c* respectively. Curve *a* shows the expected atomic energy levels split by crystal-field theory and *b* shows these levels convoluted by a 0.8 eV broad Gaussian to simulate the instrumental resolution [79J].