substance: MnO
property: band structure, energy gap

Brillouin zone: Fig. 1, partial APW band structure: Fig. 2. This calculation overestimates the O 2p – Mn 3d energy separation [78K].

energy gaps

$E_{g,th}$	2.43(8) eV		from transport data	67H
	2.6 eV			68A
	2.6(2) eV			71G
	$1.90–6\cdot10^{-4}T$ eV		T in K	76K
	2.7...3.0 eV		from photoconductivity, Fig. 3	77U
E_g	3.6 eV	T = 300 K	from UV absorption; shift of 500 cm^{-1} in E_g below T_N	74C

References:

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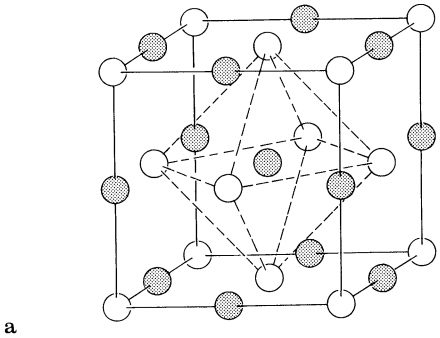
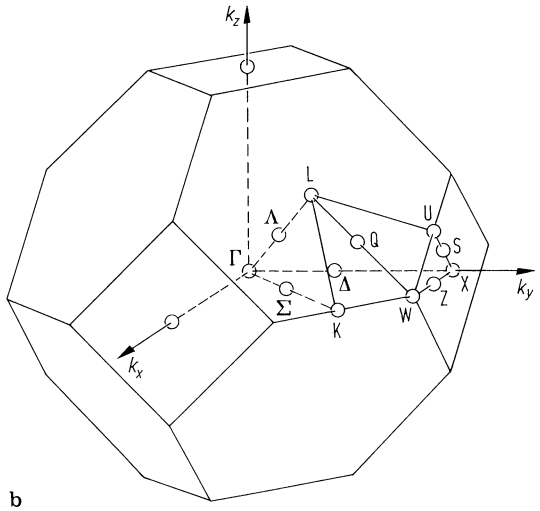
68A Ali, M., Fridman, M., Denayer, M., Nagels, P.: Phys. Status Solidi 28 (1968) 193.
71G Gvishi, M.: Solid State Commun. 9 (1971) 2089.
72M Mattheiss, L. F.: Phys. Rev. B5 (1972) 290.
74C Chou, H. H., Fan, H. Y.: Phys. Rev. B10 (1974) 901.
76K Kleinpenning, T. G. M.: J. Phys. Chem. Solids 37 (1976) 925.
77U Usani, T., Masumi, T.: Physica 86-88 B+C (1977) 985.
78K Kunz, A. B., Surratt, G. T.: Solid State Commun. 25 (1978) 9.

Fig. 1.

MnO. Unit cell (a) and Brillouin zone (b) for the face centered cubic lattice.



a



b

Fig. 2.

3d-monoxides. Energy band structure obtained by an APW calculation plotted along the Δ-direction [72M].

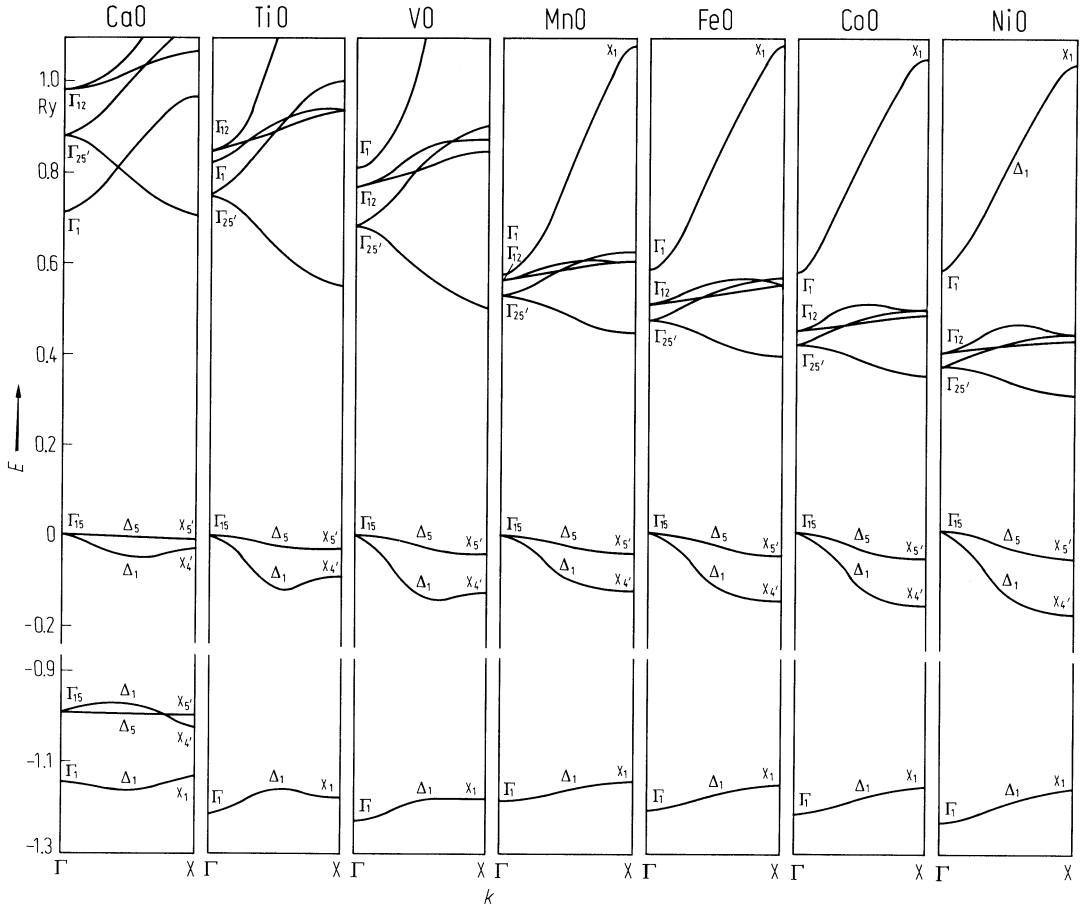


Fig. 3.

MnO. Photocurrent vs. wavelength of exciting light for various crystals *1* as grown, *2* annealed in p_{CO_2}/p_{H_2} = 0.1, *3* annealed in p_{CO_2}/p_{H_2} = 1.0 [77U].