substance: V_2O_3
property: electronic properties

band structure

Two major calculations have been reported [76A, 78C] based on earlier work [71N, 71W, 73A, 75A]. The major controversy is over the ordering of the e_π and a_1 components of the trigonally split t_{2g} band. [76A] finds, on inclusion of correlation effects, that e_π lies below a_1 (Figs. 1...3), but [78C] assumes a configuration $a_1^1\ e_1$ for V_2O_3. This latter is inconsistent with the antiferromagnetic coupling observed in the low-temperature form [70G]. In monoclinic V_2O_3, the e_π band is further split into e_1 and e_2 components (Figs. 4...6).

calculated orbital occupancies

e_π	1.927	metallic phase	76A
a_1	0.073	($T > T_{tr}$)	
e_1 (↑)	0.900	semiconducting	
e_1 (↓)	0.025	phase	
e_2 (↑)	0.958	($T < T_{tr}$)	
e_2 (↓)	0.039		
a_1 (↑)	0.070		
a_1 (↓)	0.070		

Several empirical band schemes have been suggested: Fig. 7 and [70G, 72H, 76S].

References:

70G Goodenough, J. B.: Proc. 10th Int. Conf. Phys. Semicond. 1970, 304.
71N Nebenzahl, I., Weger, M.: Philos. Mag. 24 (1971) 1119.
71W Weger, M.: Philos. Mag. 24 (1971) 1095.
72H Honig, J. M., Van Zandt, L. L., Board, R. D., Weaver, H. E.: Phys. Rev. B6 (1972) 1323.
73A Ashkenazi, J., Weger, M.: Adv. Phys. 22 (1973) 207.
75A Ashkenazi, J., Chuchem, T.: Philos. Mag. 32 (1975) 763.
76A Ashkenazi, J., Weger, M.: J. Phys. 37 (1976) C4-189.
76S Shuker, P., Yacoby, Y.: Phys. Rev. B14 (1976) 2211.
78C Castellani, C., Natoli, C. R., Ranninger, J.: Phys. Rev. B18 (1978) 4945, 4967, 5001.

Fig. 1.

V_2O_3. Energy dispersion in the t_{2g}-band of metallic V_2O_3 [76A].

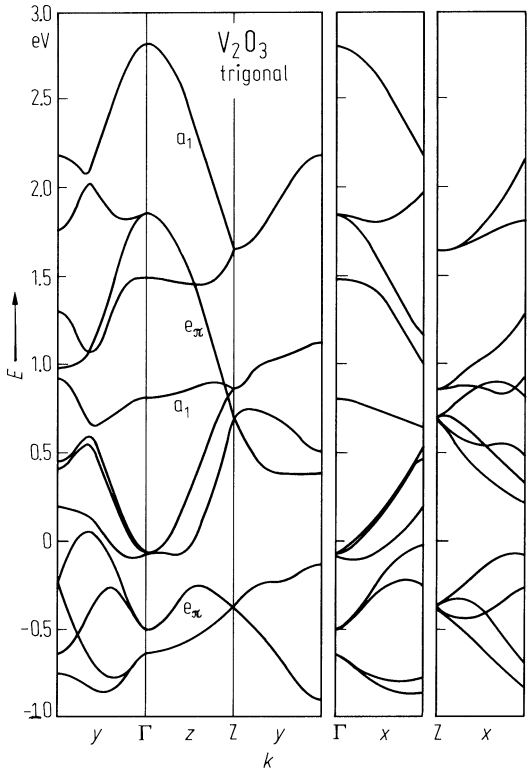

Fig. 2.

V_2O_3. Density of states in the t_{2g}-band of metallic V_2O_3 [76A].

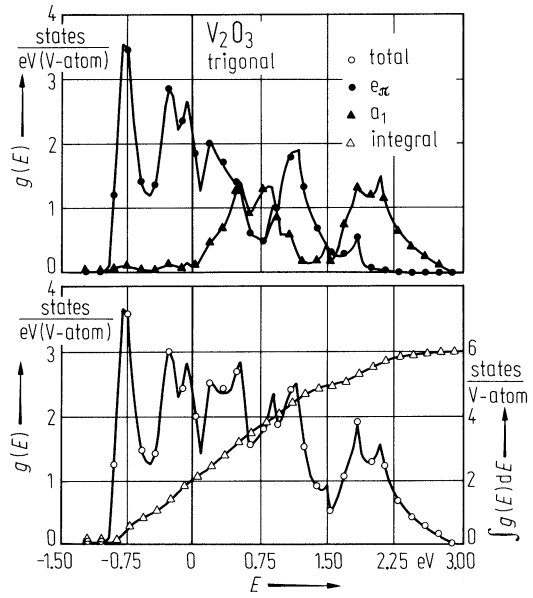

Fig. 3.

V_2O_3. Joint density of states in metallic V_2O_3 [76A].

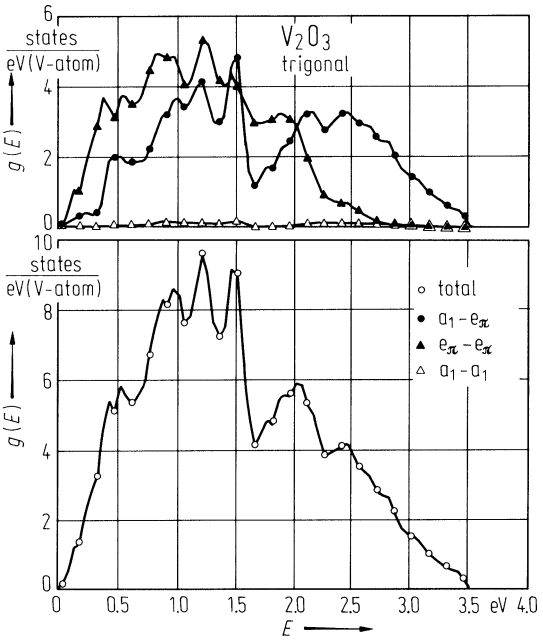

Fig. 4.

V_2O_3. Ferromagnetic and antiferromagnetic chains [76A].

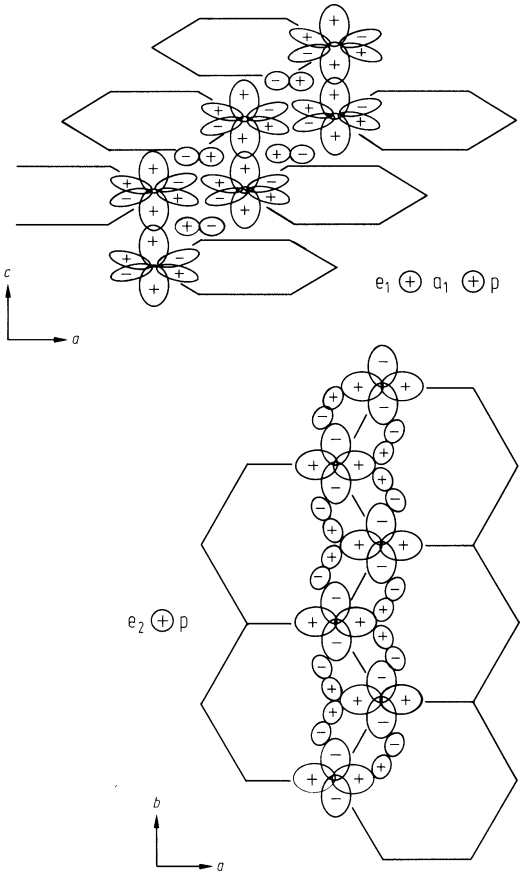

Fig. 5.

V_2O_3. Energy dispersion in the t_{2g}-band of monoclinic V_2O_3; the arrows indicate the direction of the magnetic moments on sites where a spin-up state of the band is concentrated [76A].

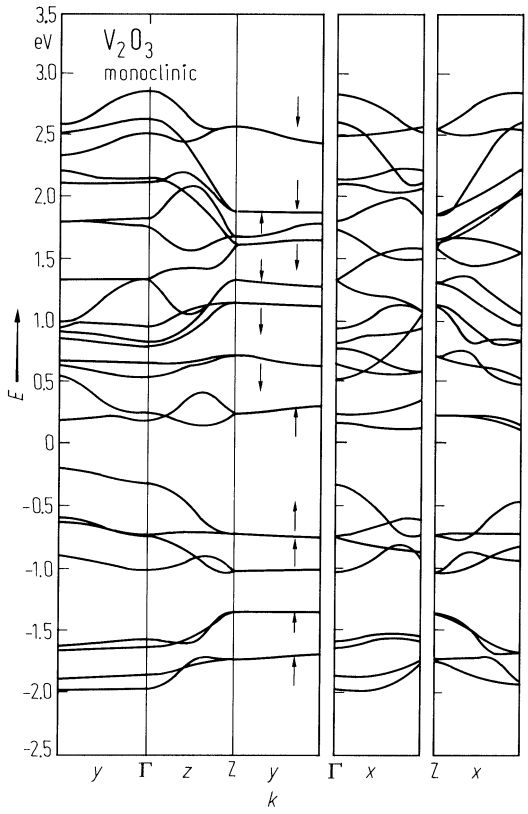

Fig. 6.

V_2O_3. Density of states in monoclinic V_2O_3 [76A].

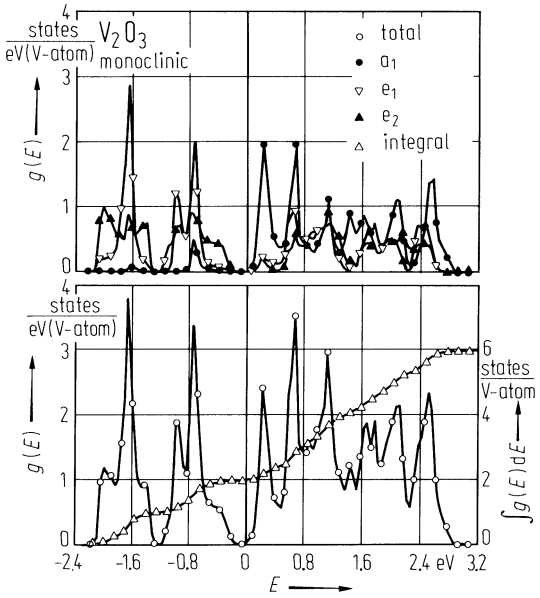

Fig. 7.

V_2O_3. Empirical band schemes: (a) [70G], (b) [72H], (c) HT - LT transition [70G, 76S]. Numbers in brackets indicate number of band states per molecule.