substance: MnO
property: optical properties

higher energy peaks in the optical spectra

Photoemission spectrum, decomposed into Mn 3d and O 2p components: Fig. 1. The spectrum can be understood in terms of ionization of local Mn^{2+} electrons to give ^5E and $^5T_2$ states separated by 1.56 eV and broadened by Franck-Condon factors.

peak wavenumbers in optical spectra

For spectra, see Fig. 2 and [69H1, 69H2, 59P]

$(\nu/c)_{peak}$	15532 cm^{-1}	band 1, transition $^6A_{1g} - {}^4T_{1g}(I)$	77Y
	ca. 19000 cm^{-1}	band 2, transition $^6A_{1g} - {}^4T_{2g}(I)$	
	23322 cm^{-1}	band 3, transition $^6A_{1g} - {}^4A_{1g}$	
	23389 cm^{-1}	transition $^6A_{1g} - {}^4E_g(I)$	
	25659 cm^{-1}	band 4, transition $^6A_{1g} - {}^4T_{2g}(II)$ fine structure associated with these peaks was assigned to a magnon side band at 112 cm^{-1} and optical phonons	
	29000 cm^{-1}	interband absorption edge, see Fig. 3; assigned to Mn 3d – Mn 4s	74C

peak energies in reflectance spectra

E_{peak}	4 eV	RF, T = 300 K	onset of reflectance	76K,
			RF: reflectance spectrum, TF: thermoreflectance	72M
	4.6 eV	RF, T = 22 K	assignment: Mn e_g – Mn 4s	
	4.7 eV	RF, T = 300 K		
	4.9 eV	TF, TI	TI: temperature independent; thermoreflectance spectrum Fig. 4; derived empirical band diagram: Fig. 5	
	5.2 eV	RF, T = 22 K		
	5.4 eV	TF,TI	Mn e_g – Mn t_{2g}	
	5.5 eV	RF, T = 22 K	Mn t_{2g}-Mn 4s	
	5.7 eV	TF, T = 85 K	shifted to 5.55 eV at 200 K O 2p – Mn 4s	
	6.3 eV	RF, T = 22 K	Mn e_g – Mn e_g; Mn t_{2g} – Mn t_{2g}	
	6.4 eV	TF, TI		
	6.6 eV	RF, T = 300 K	peak at 22 K, shoulder at 300 K	
	6.9 eV	RF, T = 300 K	alsoTF, O 2p – Mn 4s	
	7.0 eV	TF, T = 200 K	shifts to 6.7 eV at 310 K	
	7.2 eV	RF, T = 22 K	Mn t_{2g} – Mn e_g	
		TF, TI		
	4...7.5 eV	T = 300 K	Mn e_g – Mn t_{2g}	76K
	8...10.6 eV	T = 300 K	Mn t_{2g} – Mn 4s	
	11...19 eV	T = 300 K	O 2s – Mn 4s	
	16(1) eV	RF, T = 22 K		72M
	5.3 eV	RT	EELS data O 2p – Mn t_{2g}	78A
	8.2 eV		O 2p – Mn e_g	
	9.8 eV		O 2p – Mn 4s	

References:

59P Pratt, G. W., Coelho, R.: Phys. Rev. 116 (1959) 281.
69H1 Haywood, B. C. G., Collins, M. F.: J. Phys. C2 (1969) 46.
69H2 Huffmann, D. R., Wild, R. L., Shinmei, M.: J. Chem. Phys. 50 (1969) 4092.
72M Messick, L., Walker, W. C., Glosser, R.: Phys. Rev. B6 (1972) 3941.
74C Chou, H. H., Fan, H. Y.: Phys. Rev. B10 (1974) 901.
75E Eastman, D. E., Freeouf, J. L.: Phys. Rev. Lett. 34 (1975) 395.
76K Ksendzov, Y. M., Korobova, I. L., Sidorin, K. K., Startsev, G. P.: Fiz. Tverd. Tela 18 (1976) 173.
77Y Yokogawa, M., Taniguchi, K., Hamaguchi, C.: J. Phys. Soc. Jpn. 42 (1977) 591.
78A Akimoto, K., Sakisaki, Y., Nishijama, M., Onchi, M.: J. Phys. C11 (1978) 2535.

Fig. 1.

MnO. Photoemission spectrum (intensity vs. binding energy relative to the E_d peak energy) showing estimated deconvolution into Mn 3d and O 2p; E_p and E_d denote the p- and d-band edges and the vertical lines are the calculated positions of the $3d^{n-1}$ states [75E].

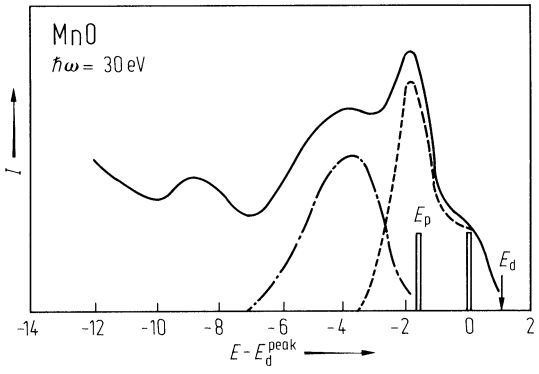

Fig. 2.

MnO. Optical density vs. photon energy (wavelength) at 300 and 78 K. Film thickness 100 μm [69H1].

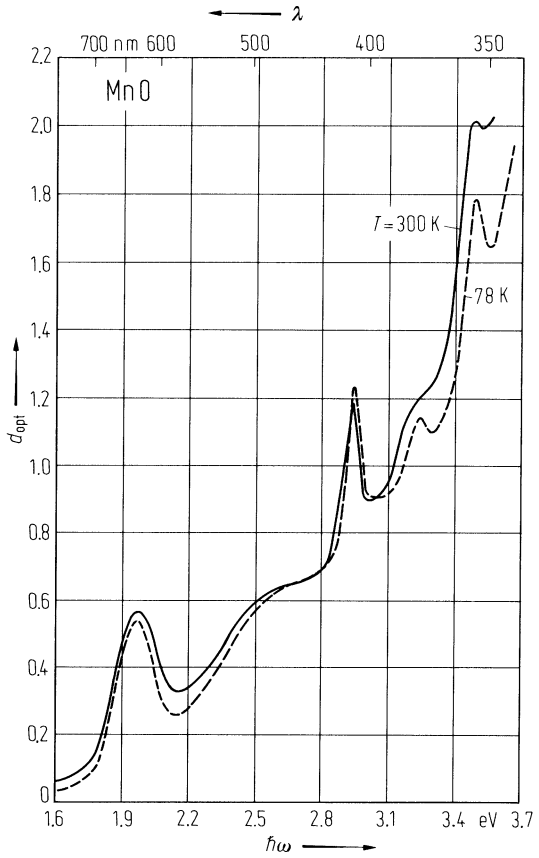

Fig. 3.

MnO. Absorption coefficient vs. wavenumber for three temperatures near the absorption edge (arrow) [74C].

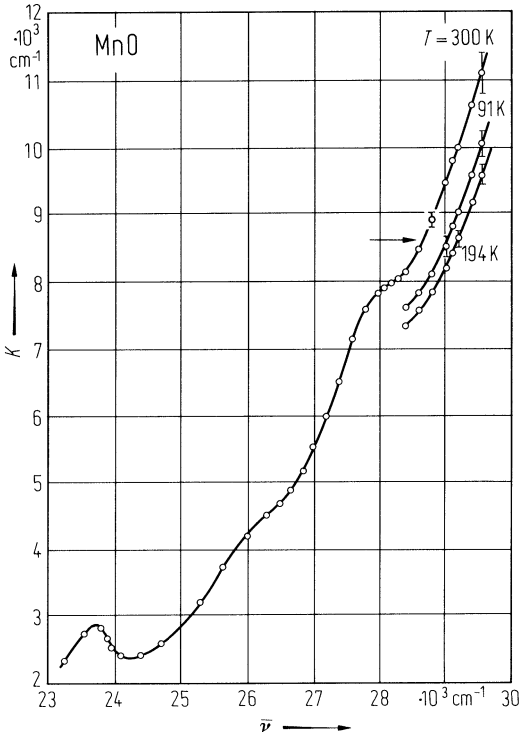

Fig. 4.

MnO. Thermoreflectance vs. wavelength (photon energy) at 85 K (lower figure) and 200 and 310 K (upper figure) [72M]. Peak positions (in eV) are indicated.

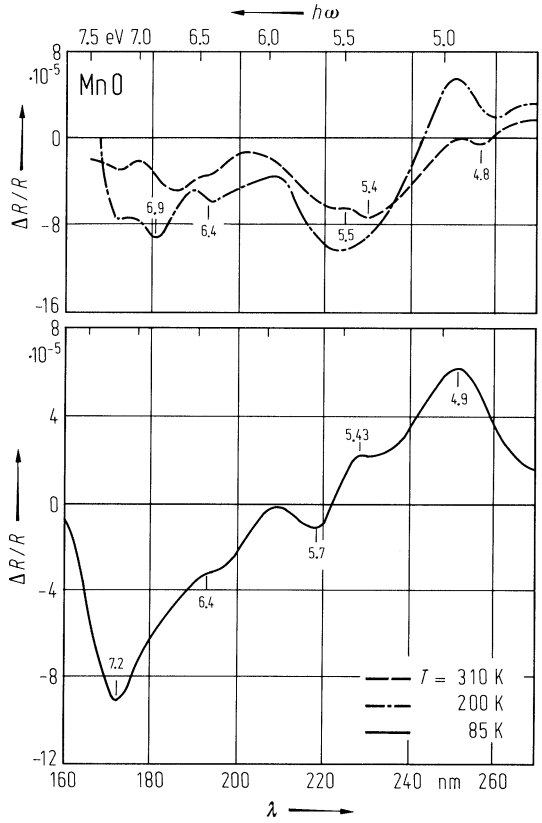

Fig. 5.

MnO. Electronic states (at RT): one-electron bands are shown on the left and localized states on the right [72M]. I: $d^4(t_\alpha^3 e_\alpha)$ + 4s; II: $d^4(t_\alpha^3 e_\alpha)$ + $d^6(t_\alpha^3 t_\beta e_\alpha^2)$; III: $d^4(t_\alpha^2 e_\alpha^2)$ + 4s; IV: $d4(t_\alpha^3 e_\alpha)$ + $d^6(t_\alpha^3 e_\alpha^2 e_\beta)$ and $d^4(t_\alpha^2 e_\alpha^2)$ + $d^6(t_\alpha^3 t_\beta e_\alpha^2)$; V: $d^4(t_\alpha^2 e_\alpha^2)$ + $d^6(t_\alpha^3 e_\alpha^2 e_\beta)$.