substance: V_2O_5
property: optical properties

optical spectra: electroreflectance and ε_2 spectra: Figs. 1, 2, reflectivity in the far UV: Fig. 3 (other reflectivity data: [73V, 72M, 69M]), absorption coefficient near the band edge: Fig. 4.

absorption coefficient

In the sub-bandgap region K shows a strong Urbach tail $K = K_0 \exp(\beta h\nu/kT)$ with $\beta = 0.55$ for $E \parallel a$ and 0.52 for $E \parallel c$ [66K], $\beta = 0.50$ ($E \perp c$) and 0.47 ($E \parallel c$) [67B]. Strong absorption is found for $E \parallel a$ at 1.24 eV with a shoulder at 1.50 eV which derive from defect centres. Careful studies [74C, 78V] have shown that this F1 absorption is due to electrons trapped at or near an oxygen vacancy. The EPR principal axes are coplanar with the layers in V_2O_5, but the x and z axes lie at 25° to the c and a axes of the crystal and a fit to a two-electron centre is found with electrons located on 2 or 3 nearest neighbour vanadium atoms.

energies of experimental absorption maxima

a, b, c indicate the polarization, the three columns to the right give the corresponding energies and (in brackets) oscillator strengths (10^{-2}) for the cluster models mentioned in the documents on electronic properties for n = 4, 5 and 6 respectively. (Table from [77L].)

			n = 4			n = 5			n = 6		
E (in eV)	2.17	(a)	2.92	(0.12)	(a)	2.79	(2.34)	(a)	2.18	(0.084)	(a)
										(1.33)	(b)
	2.2	(a)	3.03	(0.26)	(a)	2.00	(0.68)	(a)	2.55	(0.36)	(a)
										(3.93)	(b)
	2.5	(a)	3.14	(0.55)	(c)	3.30	(0.77)	(a)	2.71	(0.74)	(a)
	2.54	(c)	3.31	(0.15)	(a)	3.50	(1.52)	(c)	2.89	(3.68)	(a)
	2.9	(a)	3.31	(0.53)	(c)	3.69	(1.98)	(a)	3.05	(4.91)	(a,b)
	3.0	(c)	3.49	(0.43)	(c,b)	4.39	(1.29)	(a)	3.17	(0.71)	(c)
	3.25	(c)	3.68	(0.42)	(a,b)	4.51	(2.63)	(c)	3.25	(0.39)	(c)
	3.38	(a)	3.88	(0.52)	(a,b)	4.66	(2.05)	(a,b)	3.45	(1.41)	(b,c)
	3.7	(c)	3.89	(0.47)	(c)	4.68	(1.63)	(c)	3.75	(3.04)	(a)
	3.87...3.9	a)	4.18	(1.86)	(c)	4.85	(1.07)	(a,b)	4.26	(1.89)	(a)
	4.15	(c)	4.41	(2.25)	(a)	5.00	(0.47)	(a,b)	4.59	(1.8)	(a)
	4.4	(a)	4.76	(1.71)	(a)	5.16	(0.39)	(a)	4.72	(1.23)	(a,b)
	4.9	(c)	5.12	(0.36)	(a)	5.82	(1.42)	(a)	4.80	(1.40)	(c)
	5.3	(a)	5.60	(1.35)	(a,b)				5.06	(1.48)	(c)
	6.5	(a,c)							5.13	(2.49)	(a)

refractive index

$n(\infty)$	2.07	$E \parallel a$	parameters of the equation	66K
A	0.284 μm^2		$n = n(\infty) + A\,\lambda^{-2}$ (λ in μm)	
$n(\infty)$	1.97	$E \parallel b$		
A	0.045 μm^2			
$n(\infty)$	2.12	$E \parallel c$		
A	0.149 μm^2			

ESR data on $W_xV_2O_5$ show two defects. One is intrinsic to V_2O_5 and derives from oxygen vacancies whereas the other is derived from $W^{6+} - O - V^{4+}$ units [81G].

References:

66K Kenay, N., Kannewurf, O. R., Whitmore, D. H.: J. Phys. Chem. Solids 27 (1966) 1237.
67B Bodó, Z., Hevesi, I.: Phys. Status Solidi 20 (1967) K45.
69M Mokerov, V. G., Rakov, A. V.: Fiz. Tverd. Tela 11 (1969) 197.
72M Mokerov, V. G., Sigelov, B. L.: Fiz. Tverd. Tela 14 (1972) 3405.
73V Valiev, K. A., Mokerov, V. G., Rakov, A. V.: Fiz. Tverd. Tela 15 (1973) 361.
74C Clauws, P., Vennik, J.: Phys. Status Solidi (b) 66 (1974) 553, 953.
76V Volzhenski, D. S., Grin', V. A., Savitskii, V. G.: Kristallografiya 21 (1976) 1238.
77L Lazukova, N. I., Gubanov, V. A., Mokerov, V. G.: Int. J. Quantum Chem. 12 (1977) 915.
78V Vanhaelet, M., Clauws, P.: Phys. Status Solidi (b) 87 (1978) 719.
81G Gaillard, B., Blanchard, C., Deville, A., Livage, J.: Phys. Status Solidi (b) 104 (1981) 627.

Fig. 1.

V_2O_5. Electroreflectivity and imaginary part of the dielectric constant vs. photon energy for $E \parallel a$. Arrows mark peak positions in the reflectance spectrum [77L].

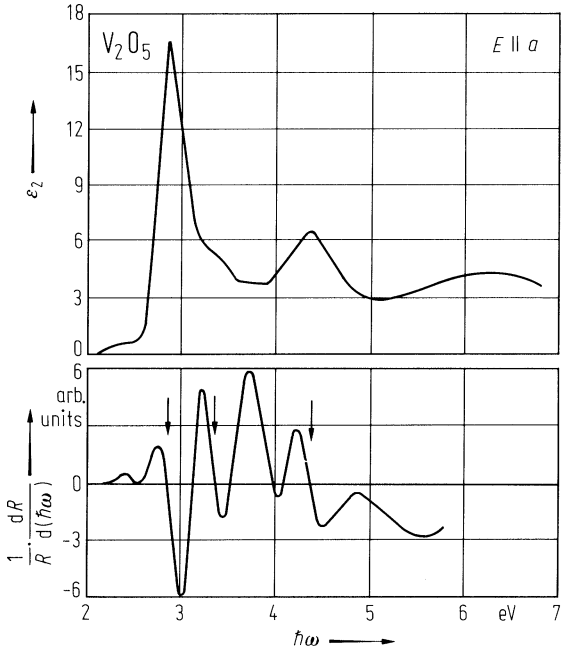

Fig. 2.

V_2O_5. Electroreflectivity and imaginary part of the dielectric constant vs. photon energy for $E \parallel c$. Notation as in Fig. 1 [77L].

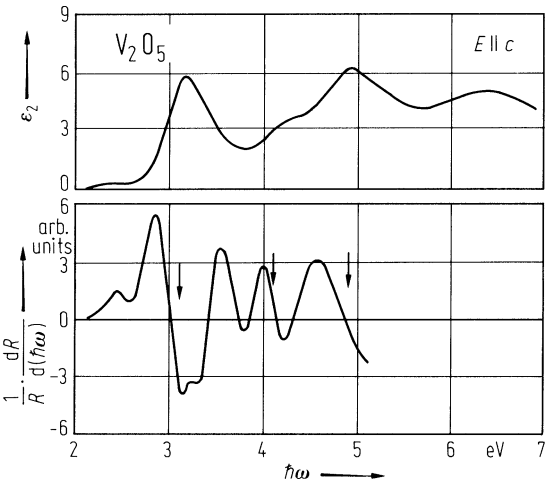

Fig. 3.

V_2O_5. Reflectivity vs. photon energy [77L]. Peak positions are indicated.

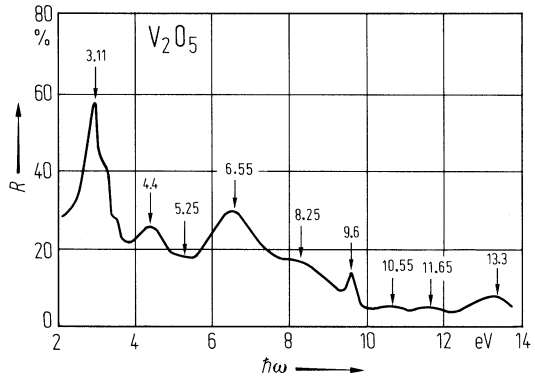

Fig. 4.

V_2O_5. Absorption coefficient vs. photon energy for $E \parallel c$ (open circles) and $E \parallel b$ (full circles) [76V]. K in cm^{-1}.