substance: $Zr_{1+x}Se_2$
property: crystal structure, physical properties

$Zr_{1+x}Se_2$ ($0.05 \leq x \leq 0.08$)

Data from [58M, 65G, 69L, 73B, 78B]

(S: structure (space group), CG: crystal growth (the numbers in parentheses correspond to T_1 and T_2, the temperatures (in °C) of the hot and cold end of the crystal growth tube, respectively), C: colour).

lattice parameters

a	3.76 Å	S: C6, $D_{3d}^3 - P\bar{3}m1$
c	6.15 Å	CG: halogen transport (900/800)
		C: metallic grey

resistivity, Seebeck coefficient

ρ	0.1 Ω cm	n-type, poly-
S	– 300 μV K^{-1}	crystalline sample

energy gap

E_g	0.87 eV	$Zr_{1.05}Se_2$	optical gap
	1.2 eV	$ZrSe_2$	optical gap
	1.0 eV		indirect gap, calculated

Figures to this document:

Brillouin zone: Fig. 1b

reflectivity: Fig. 2

band structure, density of states: Fig. 3

References:

78B Bullett, D. W.: J. Phys. C 11 (1978) 4501.
58M McTaggart, F. K.: Aust. J. Chem. 11 (1958) 471.
65G Greenaway, D. L., Nitsche, R.: J. Phys. Chem. Solids 26 (1965) 1445.
69L Lee, P. A., Said, G., Davis, R., Lim, T. H.: J. Phys. Chem. Solids 30 (1969) 2719.
73B Brattas, L., Kjekshus, A.: Acta Chem. Scand. 27 (1973) 1290.

Fig. 1.

TiS_2. (a) Band structure and density of states. (b) Brillouin zone [78B].

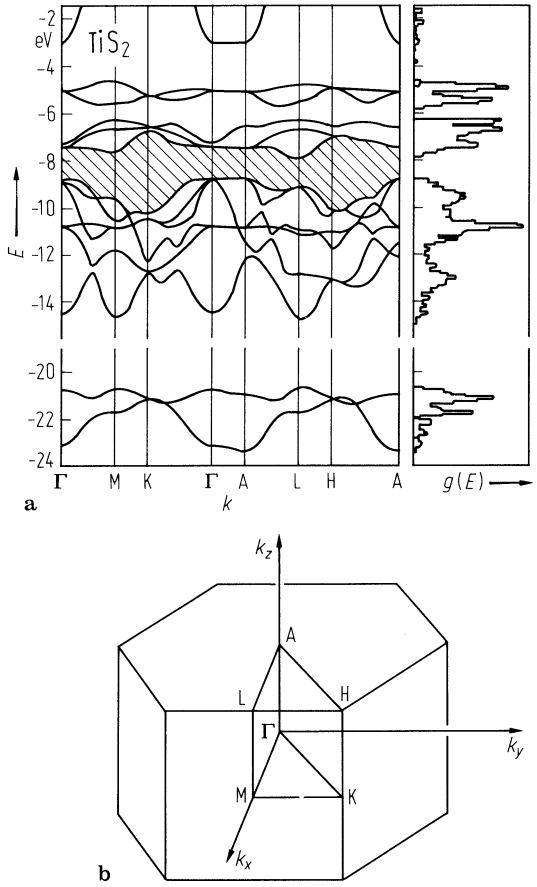

Fig. 2.

$ZrSe_2$. Reflectivity vs. photon energy in the fundamental region at room temperature [65G].

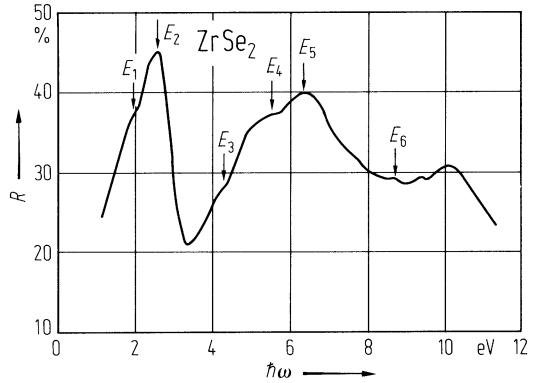

Fig. 3.

$ZrSe_2$. Band structure and density of states [78B]. See Fig. 1b for Brillouin zone.