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

$Ti_{1+x}Se_2$ ($0 \le x \le 0.018$)

(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).

(The references in the last column refer to all data of this document)

lattice parameters

a	3.537 Å		S: C6, $D_{3d}^3 - P\bar{3}m1$	76D,
c	6.00 Å		second-order phase transition at T_{tr} = 200 K, $T < T_{tr}$: transverse atomic displacements with $\boldsymbol{q}$ = (1/2, 0, 1/2)	77F, 78B, 78Z
			CG: halogen transport (900/≤800) C: metallic	

resistivity

$\rho_\perp$	$1.32\cdot10^{-3}$ Ω cm	p-type, synthetic single crystal	$d\rho/dp < 0$
$\rho_\parallel$	$3\cdot10^{-3}$ Ω cm		

Seebeck coefficient

$S_\perp$	20 µV K^{-1}	p-type synthetic single crystal	n-type for $T < T_{tr}$

Hall coefficient

R_H ($B\parallel c$)	$3.25\cdot10^{-2}$ cm^3/C	p-type synthetic single crystal	$dR_H/dp < 0$

hole concentration

p	10^{20} cm^{-3}

energy gap

E_g	≈ 0.0 eV	optical gap (semimetal)
	0.0 eV	calculated

Figures to this document:

resistivity: Figs. 1, 3

Hall coefficient, Seebeck coefficient: Fig. 2

reflectivity: Fig. 4

band structure: Fig. 5

References:

65G Greenaway, D. L., Nitsche, R.: J. Phys. Chem. Solids 26 (1965) 1445.

76D DiSalvo, F. J., Moncton, D. E., Waszczak, J. V.: Phys. Rev. B14 (1976) 4321.

77F Friend, R. H., Jerome, D., Liang, W. Y., Mikkelsen, J. C., Yoffe, A. D.: J. Phys. C 10 (1977) L705.

78B Bullett, D. W.: J. Phys. C 11 (1978) 4501.

78Z Zunger, A., Freeman, A. J.: Phys. Rev. B17 (1978) 1839.

Fig. 1.

$TiSe_2$. Electrical resistivity perpendicular to the *c* axis (parallel to the layers) for crystals grown by iodine vapor transport at different growth temperatures (T_g). The bar on the curve for T_g = 575ºC represents the spread in peak values observed in crystals from the same bath [76D].

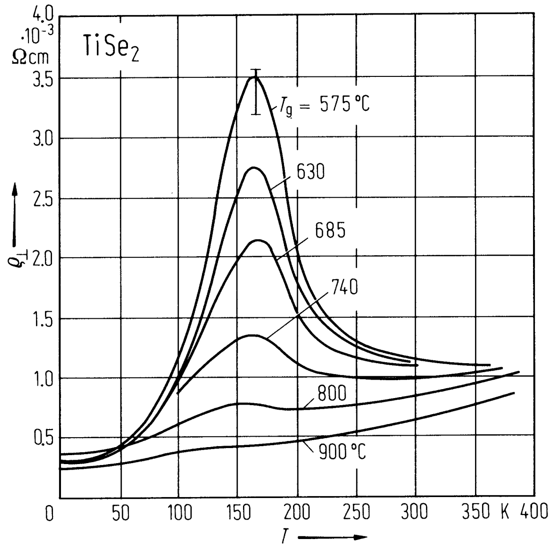

Fig. 2.

$TiSe_2$. Hall coefficient and thermoelectric power perpendicular to *c* axis vs. temperature [76D].

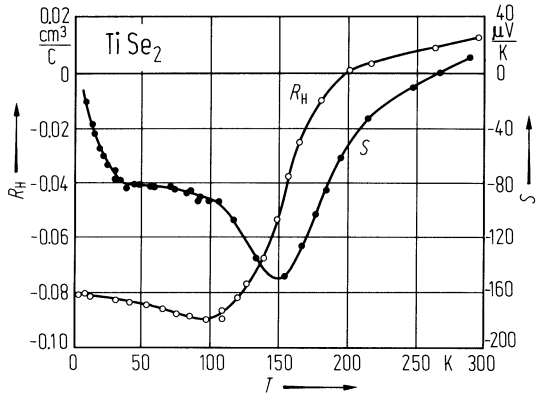

Fig. 3.

$TiSe_2$. Electrical resistivity vs. temperature perpendicular to the *c* axis (a) and parallel to the *c* axis (b) for sublimation-grown (at 630°C) $TiSe_2$. The insets show dρ/dT for the same sample [76D].

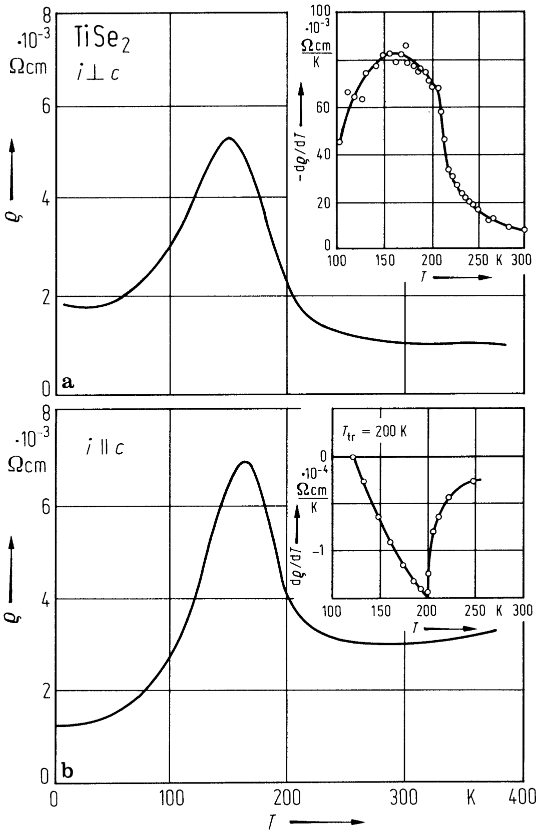

Fig. 4.

$TiSe_2$. Reflectivity vs. photon energy in the fundamental region at room temperature [65G].

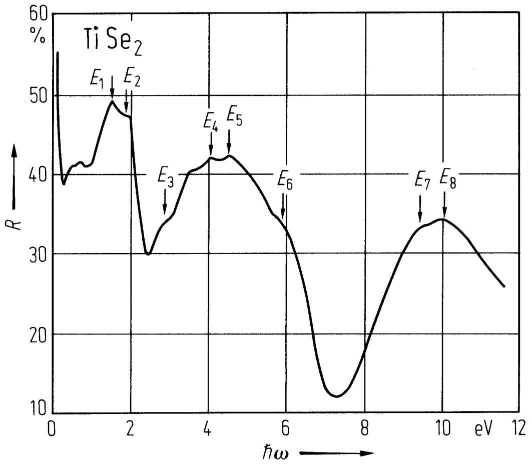

Fig. 5.

$TiSe_2$. Energy-band structure in the local exchange and correlation model [78Z].