substance: $Ti_{1+x}S_2$
property: crystal structure, physical properties

$Ti_{1+x}S_2$ ($0 \le x \le 0.1$)

(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).

Data from [63H, 65G, 67G, 68C, 69L, 72T, 75C, 75T1, 75T2, 75W, 77F, 78B, 83H]

			at 1000°C: $0.04 \le x \le 0.1$ at 500°C: $0.03 \le x \le 0.1$ at 600°C: $0 \le x \le 0.1$

lattice parameters

a	3.407 Å	$x \approx 0$	S: C6, $D_{3d}^3 - P\bar{3}m1$
c	5.695 Å		CG: halogen transport (900/800)

density

d	3.22 g cm^{-3}		C: brassy

resistivity

$\rho_\perp$	$5 \cdot 10^{-3}$ Ω cm	n-type, synthetic single crystal	$d\rho/dp < 0$
$\rho_a = \rho_0 + \rho_1 T^2 = 1.95 \cdot 10^{-4}$ Ω cm $+ (2.0 \cdot 10^{-8}/k^2 T^2)$ [Ω cm]			$\rho_1 \propto n^{-5/3}$, where n = carrier concentration; shows electron-electron scattering is dominant

Seebeck coefficient

$S_\perp$	– 265...– 40 μV K^{-1}	$0 \le x \le 0.1$

Hall mobility

$\mu_{H\perp}$	9.7 cm^2/V s	$dR_H/dp = 0$

electron concentration

n	$9 \cdot 10^{20}$ cm^{-3}

effective electron mass

m_n	1.5 m_0

***g*-factor**

g	4.3

energy gap

E_g	0.7eV	optical gap
	0.7 eV	indirect gap, calculated

linear thermal expansion coefficient

α_a	$0.96 \cdot 10^{-5}\ K^{-1}$	
α_c	$1.94 \cdot 10^{-5}\ K^{-1}$	

magnetic susceptibility

χ_m	$10^{-5}\ cm^3 mol^{-1}$	χ_m in CGS-emu

Figures to this document:

phase diagram, cell parameters: Figs. 1, 2

electrical conductivity: Fig. 3

Hall mobility: Fig. 4

reflectivity: Fig. 5

band structure, density of states: Fig. 6

References:

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Fig. 1.

Ti – S. Schematic pressure – composition diagram of the Ti – S system [67G]. y: atomic ratio S/Ti.

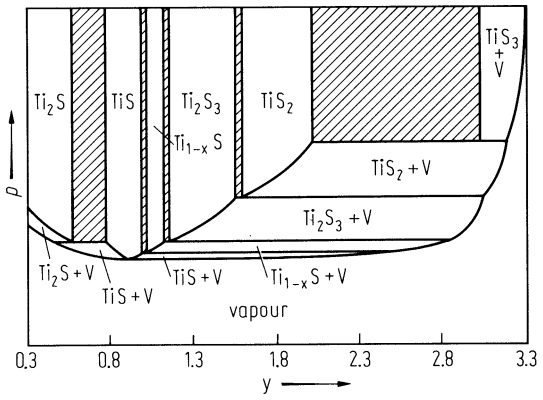

Fig. 2.

$Ti_{1+x}S_2$. Cell parameters at RT vs. composition. Sulfides prepared at 1000°C (a) and 800°C (b) [63B]. y: atomic ratio S/Ti.

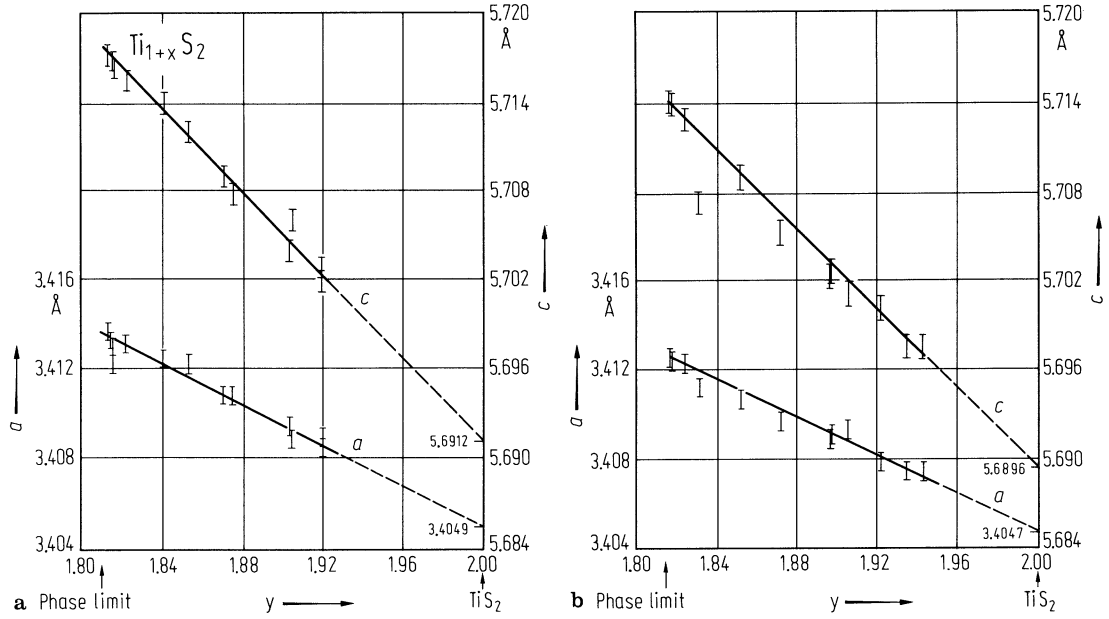

Fig. 3.

TiS_2. Electrical conductivity ($\sigma \perp c$) vs. (reciprocal) temperature for a single crvstal [68C].

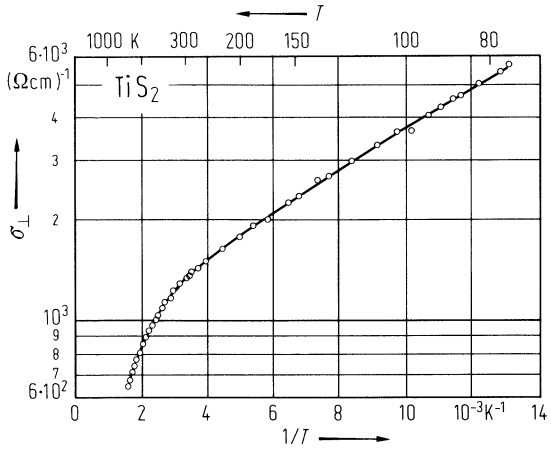

Fig. 4.

TiS_2. Hall mobility vs. temperature [68C].

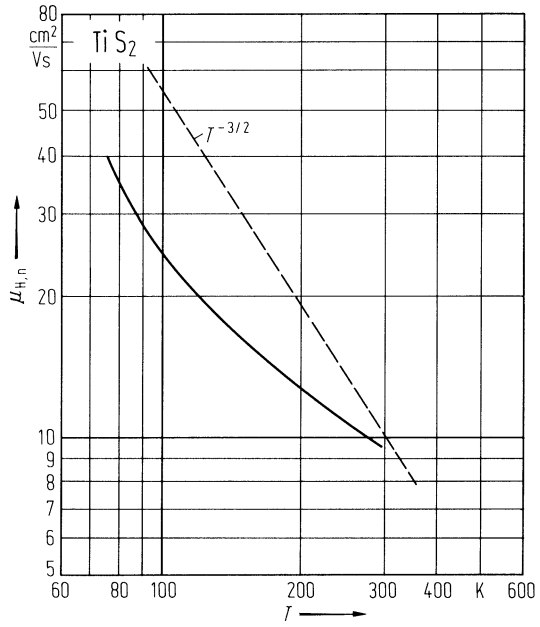

Fig. 5.

TiS_2. Reflectivity vs. photon energy in the fundamental region at room temperature [65G].

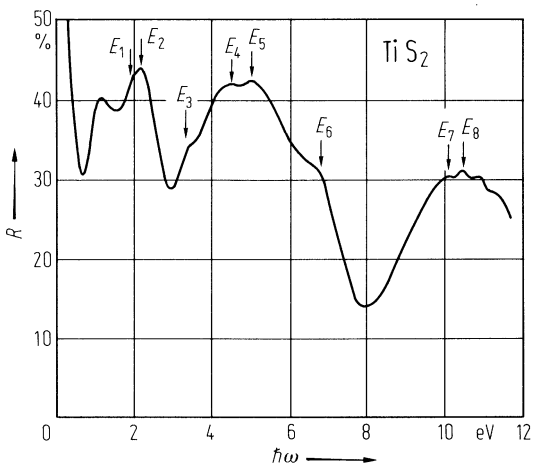

Fig. 6.

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