substance: TaS_2
property: crystal structure, physical properties

1T-TaS_2

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

(The references given in the right column refer to all data given in this document)

lattice parameters

a	3.365 Å	(modified by	S: C6, D_{3d}^3 – P$\bar{3}$m1. First-order	71C,
c	5.853 Å	formation	semiconductor-semiconductor	71T,
		of charge	transition at T_d = 150...200 K,	72C,
		density	first-order semiconductor-metal	73M,
		waves)	transition at $T_{d'}$ = 325...350 K	74G,
			$dT_{d'}/dp$ = – 3.48 K/kbar,	74W,
			$dT_d(\uparrow)/dp$ = – 5.65 K/kbar,	75S,
			$dT_d(\downarrow)/dp$ is non-linear, curve	75W1,
			fitted to $182(1–(p/5.7))^{1/2}$,	75W2,
			p in kbar. ↑ and ↓ correspond	76W,
			to heating and cooling, respectively	77D,

resistivity 77T,

ρ_a	10^{-3} Ω cm	n-type	CG: halogen transport (920/820)	77W,
		synthetic single		77Y,
		crystal	C: golden yellow	79I,

Hall coefficient, electron concentration 80J,

R_H ($B \parallel c$)	– 10^{-3} cm^3/C	80S,
n	10^{22} cm^{-3}	83H

Seebeck coefficient

S_a	– 9.5 μV K^{-1}	
	+ 3.1 μV K^{-1}	T = 363 K

energy gap

E_g	2.3 eV		calculated
$E_{g,th}$	$2\cdot10^{-4}$ eV	5 K < T < 140 K	
	$4\cdot10^{-2}$ eV	250 K < T < 340 K	

Figures to this document:

resistivity: Fig. 1

Hall coefficient, Hall mobility: Figs. 2, 3

phase diagram: Fig. 4

Fermi surface: Fig. 5

References:

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Fig. 1.

TaS_2, $TaSe_2$. Electrical resistivity vs. temperature for 1T–TaS_2 and 1T–$TaSe_2$ [77D]. $\rho \perp c$.

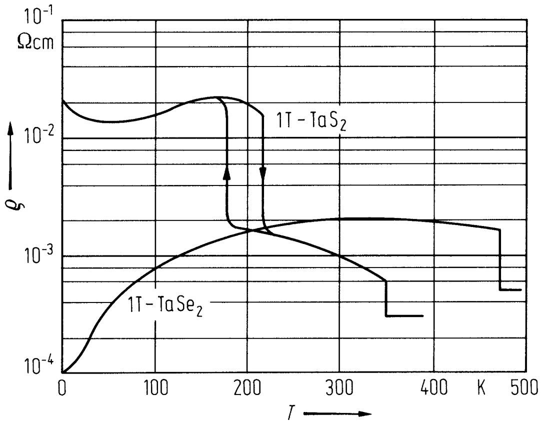

Fig. 2.

TaS_2. Hall coefficient vs. temperature in 1T–TaS_2. The lower scale on the vertical axis is enlarged five hundred times as compared with the upper one. The right-hand scale on the vertical axis gives the carrier concentration assuming a one-carrier model. Measurements on two samples [79I]. Inset shows low-temperature range on an expanded scale. $B \parallel c$.

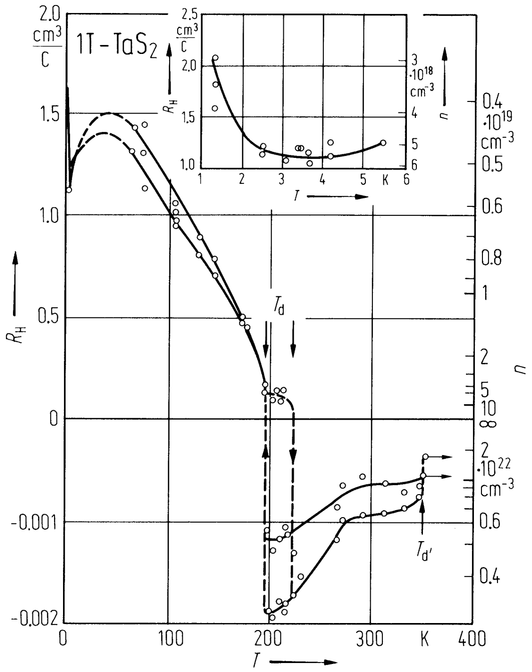

Fig. 3.

TaS_2. Hall mobility vs. temperature in 1T–TaS_2 (two samples) [79I]. $\mu \perp c$.

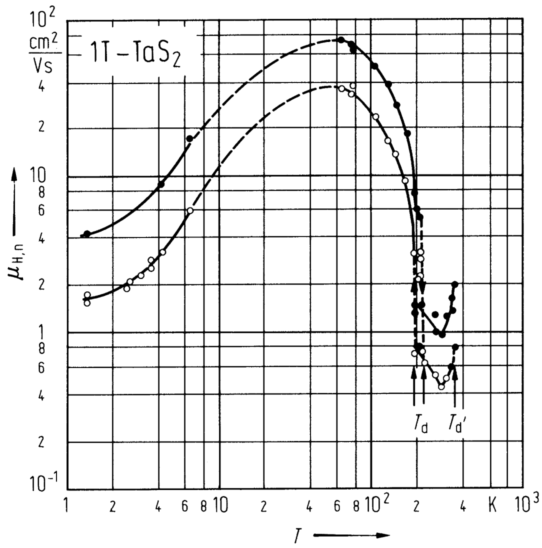

Fig. 4.

TaS_2. The phase boundary in temperature and pressure between $1T_1$– and $1T_2$–TaS_2 [74G].

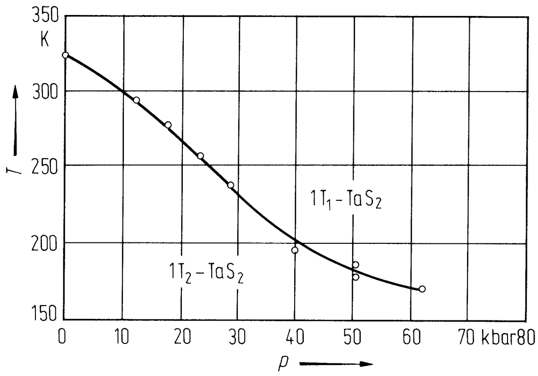

Fig. 5.

TaS_2, $TaSe_2$. (a) The Fermi surface of 1T–$TaSe_2$ in the midplane (k_z = 0) showing the direction of the spanning vector, (b) band structure of 1T–TaS_2. Circles in Γ–M are from other literature (see original paper) Error in Fig. (b): *E* values are in Ry instead of eV [77W].

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is enlarged five
one. The right-