substance: $MoTe_{2-x}$
property: crystal structure, physical properties

2H-$MoTe_{2-x}$ ($0.01 \leq x \leq 0.1$)

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

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

lattice parameters

a	3.519 Å	hexagonal	S: semiconductor-metal	66B,
c	13.964 Å	modification	transition at T_{tr}, where	70V,
a	6.33 Å	monoclinic	T_{tr} = 820°C for Te-rich	70W,
b	3.469 Å	modification	$MoTe_{2-x}$ and T_{tr} = 880°C	72A,
c	13.86 Å		for Mo-rich $MoTe_{2-x}$.	72B,
β	93°55'		$T < T_{tr}$: hexagonal,	72D,
			$D_{6h}^4 - P6_3/mmc$	75G,
			$T > T_{tr}$: monoclinic, $C_{2h}^2 - P2_1/m$	79C
			CG: halogen transport (900/700); high-temperature form halogen transport (1000/900) and water quenched	

resistivity, Seebeck coefficient, Hall coefficient, electron concentration

$\rho_\perp$	0.5...8.5 Ω cm	n-type,
$S_\perp$	– 422 µV K^{-1}	synthetic
R_H ($B \parallel c$)	– 24.17 cm^3/C	single
n	$2.6 \cdot 10^{17}$ cm^{-3}	crystal

energy gap

E_g	1.1 eV		optical gap
	1.2 eV		direct energy gap, calculated
$E_{g,th}$	1.08 eV	T > 660 K	

Figures to this document:

band structure: Fig. 1

Brillouin zone: Fig. 2

electrical conductivity, resistivity: Figs. 3, 5

Seebeck coefficient: Figs. 4, 5

References:

66B Brown, B. E.: Acta Crystallogr. 20 (1966) 268.
70V Vellinga, M. B., de Jonge, R., Haas, C.: J. Solid State Chem. 2 (1970) 299.
70W Wieting, T. J.: J. Phys. Chem. Solids 31 (1970) 2148.
72A Al-Hilli, A. A., Evans, B. L.: J. Cryst. Growth 15 (1972) 93.
72B Bromley, R. A., Murray, R. B., Yoffe, A. D.: J. Phys. CS (1972) 759.
72D Davey, B., Evans, H. L.: Phys. Status. Solidi (a) 13 (1972) 483.
75G Grant, A. J., Griffiths, T. M., Pitt, G. D., Yoffe, A. D.: J. Phys. C 8 (1975) L17.
79C Conan, A., Delaunay, D., Bonnet, A., Moustafa, A. G., Spiesser, M.: Phys. Status. Solidi (b) 94 (1979) 279.

Fig. 1.

$MoTe_2$. Band structure [72B]; see Fig. 2 for Brillouin zone, and for the meaning of P and Q. 1 Ry = 13.6 eV.

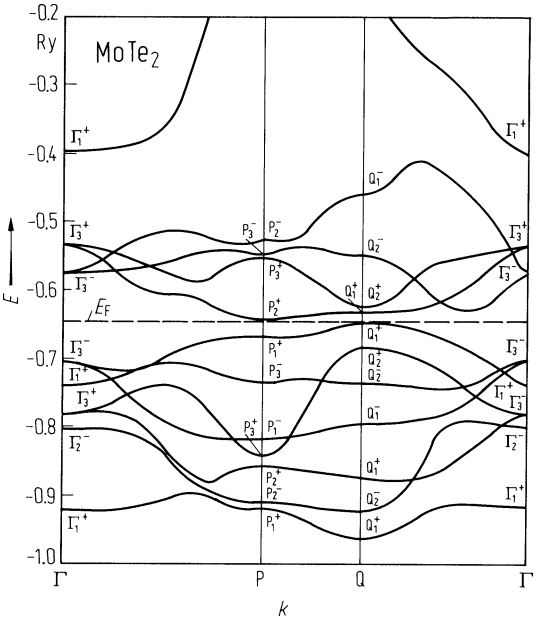

Fig. 2.

$MoSe_2$. (a) Band structure and (b) Brillouin zone for 2H-$MoSe_2$ [72B]. Q and P are the middle of each edge and the vertex of the hexagon in the two-dimensional approximation used for the calculations.

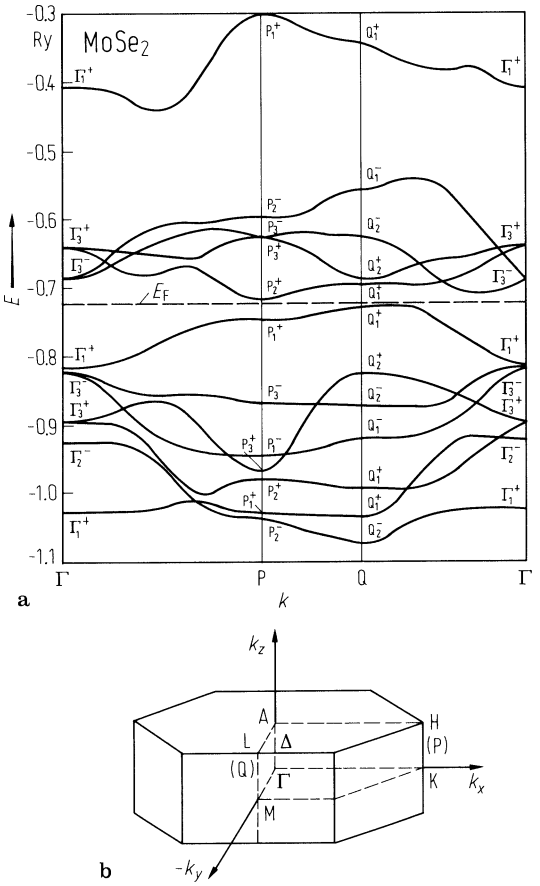

Fig. 3.

$MoTe_2$. Electrical conductivity vs. reciprocal temperature for 2H-modification. Theoretical results are drawn in full lines. *1*: monocrystalline sample, *2*: polycrystalline sample [79C]. σ in Ω^{-1} cm^{-1}, $\sigma \perp c$ (curve 1).

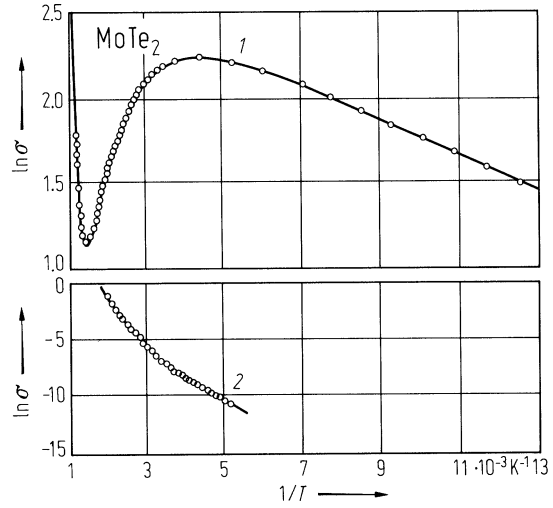

Fig. 4.

$MoTe_2$. Seebeck coefficient vs. reciprocal temperature for 2H-modification. *1*: monocrystalline sample, *2*: polycrystalline sample [79C]. $S \perp c$ (curve 1).

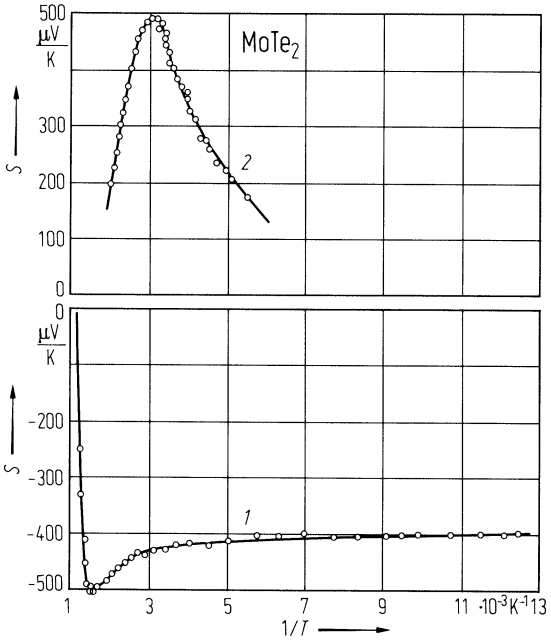

Fig. 5.

$MoTe_2$. Resistivity and thermoelectric power vs. temperature for metastable β-$MoTe_2$. The rapid increase of the resistivity at 750 K corresponds to a transition to the α-phase [70V]. Pressed-powder bar.