

**substance: ZrS<sub>2</sub>**

**property: crystal structure, physical properties**

(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 [65G, 68C, 69L, 78B, 83H]

**lattice parameters**

$a$	3.66 Å	S: C6, $D_{3d}^3 - P\bar{3}m1$
$c$	5.85 Å	CG: halogen transport (900/800)

**density**

$d$	3.87 g cm <sup>-3</sup>	C: violet metallic
-----	-------------------------	--------------------

**resistivity**

$\rho_{\perp}$	0.76 Ω cm	n-type, synthetic single crystal
----------------	-----------	-------------------------------------

**Hall mobility, electron concentration**

$\mu_{H\perp}$	4.3 cm <sup>2</sup> /V s	n-type, synthetic
$n$	$1.1 \cdot 10^{18}$ cm <sup>-3</sup>	single crystal

**energy gap**

$E_g$	1.7 eV	optical gap,
	1.7 eV	$dE_g/dT = -4.2 \cdot 10^{-4}$ eV K <sup>-1</sup> indirect gap, calculated

**Seebeck coefficient**

$S$	-700 μV K <sup>-1</sup>	n-type, polycrystalline sample
-----	-------------------------	-----------------------------------

**Figures to this document:**

**electrical conductivit** : Fig. 1

**Hall mobilit** : Fig. 2

**carrier concentratio** : Fig. 3

**reflectivit** : Fig. 4

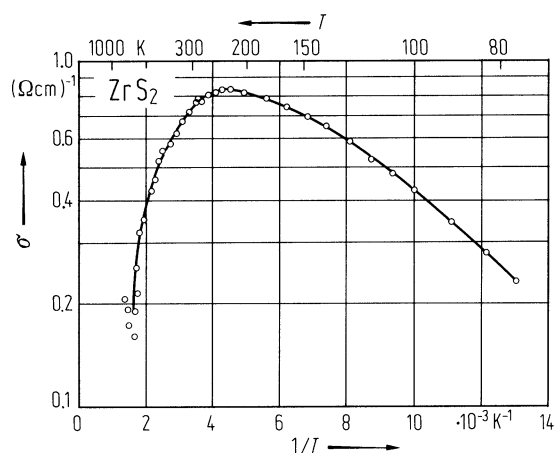
**band structur** : Fig. 5

## References:

- 65G Greenaway, D. L., Nitsche, R.: J. Phys. Chem. Solids 26 (1965) 1445.
- 68C Conroy, L. E., Park, K. C.: Inorg. Chem. 7 (1968) 459.
- 68H Hulliger, F.: Structure and Bonding, Berlin-Heidelberg-New York: Springer-Verlag 4 (1968) 83.
- 69L Lee, P. A., Said, G., Davis, R., Lim, T. H.: J. Phys. Chem. Solids 30 (1969) 2719.
- 78B Bullett, D. W.: J. Phys. C 11 (1978) 4501.
- 83H Handbook of Chemistry and Physics, 64th ed. (ed.: R. C. Weast), CRC Press. Inc. 1983.

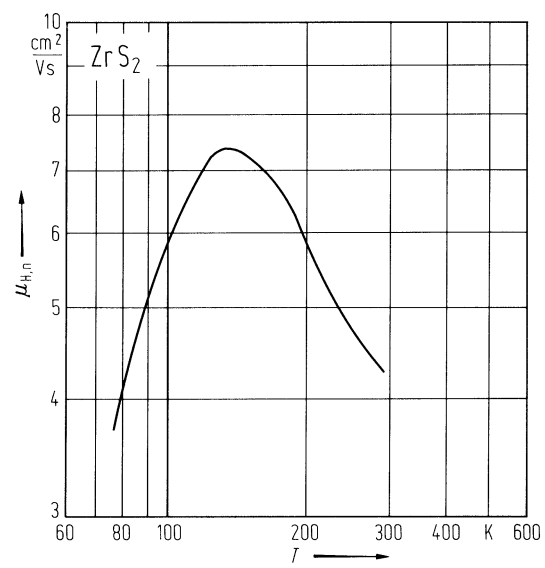
**Fig. 1.**

ZrS<sub>2</sub>. Electrical conductivity ( $\sigma \perp c$ ) vs. (reciprocal) temperature for a single crystal [68C].



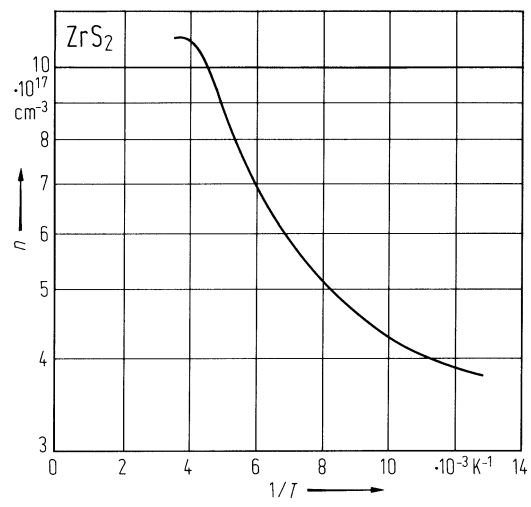
**Fig. 2.**

ZrS<sub>2</sub>. Hall mobility ( $\perp c$ ) vs. temperature [68C].



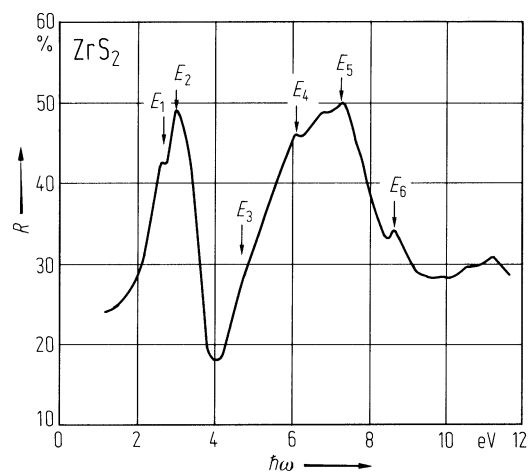
**Fig. 3.**

ZrS<sub>2</sub>. Carrier concentration vs. reciprocal temperature [68C].



**Fig. 4.**

ZrS<sub>2</sub>. Reflectivity vs. photon energy in the fundamental region at room temperature [65G].



**Fig. 5.**

ZrS<sub>2</sub>. Band structure and density of states [78B].

