**substance: $Sm_3S_4$**
**property: crystal structure, physical properties**

| | | | | |
|---|---|---|---|---|
| **crystal structure** | cubic ($Th_3P_4$-type, $T_d^6 - I\bar{4}3d$) | | | |
| **lattice parameters** | | | | |
| $a$ | 8.556 Å | | | 56P |
| | 8.5198(3) Å | | | 76B2 |
| | 8.543(2) Å | | | 79V |
| | 8.549 Å | | | 79C |
| **melting point** | | | | |
| $T_m$ | 1800°C | | | 72G |
| **linear thermal expansion coefficient** | | | | |
| $\alpha$ | $11.8 \cdot 10^{-6}$ K$^{-1}$ | | | 72G |
| **thermal conductivity** | | | | |
| $\kappa$ | $3.58 \cdot 10^{-2}$ W cm$^{-1}$ K$^{-1}$ | | | 61H |
| **phonon wavenumbers** | | | | |
| $(\nu/c)_{LO}$ | ≈ 300 cm$^{-1}$ | | Raman scattering | 77V |
| $(\nu/c)_{TO}$ | ≈ 250 cm$^{-1}$ | | | 76B1 |
| **electrical conductivity** | | | | |
| $\sigma$ | 1.8 Ω$^{-1}$ cm$^{-1}$ | | | |
| **resistivity** | | | | |
| $\rho$ | 5.9 Ω cm | | | 61H |
| | 10 Ω cm | | | 73S |
| **conduction band width** | | | | |
| $W$(5d) | 1.3 eV | | width of 5d-conduction band | 80W |
| **activation energy** | | | | |
| $E_A$ | 0.132 eV | $T > 125$ K | from electrical conductivity | 76B1, |
| | 0.142 eV | $T < 125$ K | from electrical conductivity | 76B2 |
| | 0.13 eV | | from electrical conductivity | 76E |
| | 0.1...0.2eV | | | 77V |
| | ≈ 0.1 eV | | | 77V |
| $dE_A/dp$ | 3.0(3) meV kbar$^{-1}$ | | from electrical conductivity | 76B1 |
| **Seebeck coefficient** | | | | |
| $S$ | – 150 µV K$^{-1}$ | | | 61H |

*Figures and further references:*

**mixed valence** [80H, 80W, 80M1, 80M2]

**heat capacity**: Fig. 2

**thermal conductivity**: Fig. 1

schematic **band structure:** Fig. 3

temperature dependence of **conductivity**: Fig. 4

**reflectivity spectra**: Fig. 5

electronic **Raman spectrum**: Fig. 6

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78M Merlin, R., Güntherodt, G., Humphreys, R., Cardona, M., Suryanarayanan, R., Holtzberg, F.: Phys. Rev. B 17 (1978) 4951.
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80M1 Morán-López, J. L., Schlottmann, P.: Phys. Rev. B 22 (1980) 1912.
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80W Wachter, P.: Phil. Mag. B 42 (1980) 497.

**Fig. 1.**

YbS. Temperature dependence of the thermal conductivity. Due to the small electronic contribution the total thermal conductivity is assumend to be equal to the lattice contribution [73S]. Full circles: on cooling, open circles: on heating.

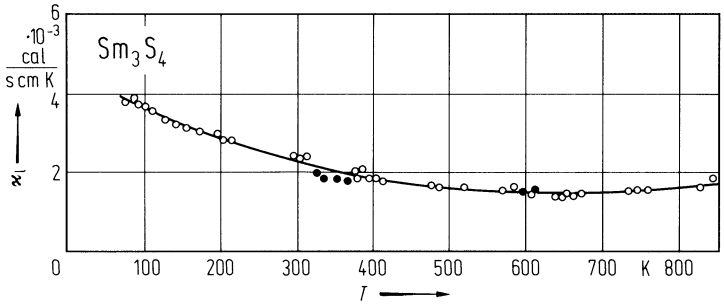


**Fig. 2.**

γ-$Sm_2S_3$, $Sm_3S_4$, $Sm_3Se_4$. Temperature dependence of molar heat capacity. The increase below 7 K is explained by a Schottky anomaly due to the crystal field splitting ($\Delta_{cf}$ = 2.4 K) of $Sm^{3+}$ [79C].

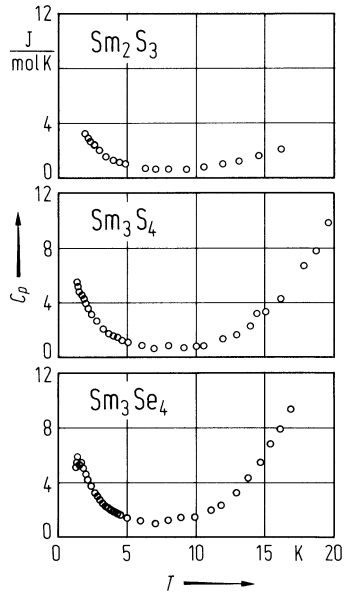


**Fig. 3.**

$Sm_3S_4$. Energy levels and schematic density of states derived from optical data [76B1]. The energy of the $4f^6$ state of $Sm^{2+}$ is chosen as zero point of energy scale. *U* is the Coulomb correlation energy.

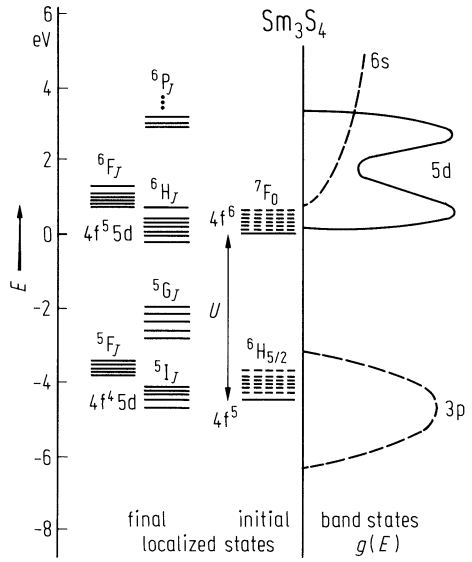


**Fig. 4.**

$Sm_3S_4$. Electrical conductivity vs. reciprocal temperature for single crystals [76B1]. Change of activation energy near 125 K.

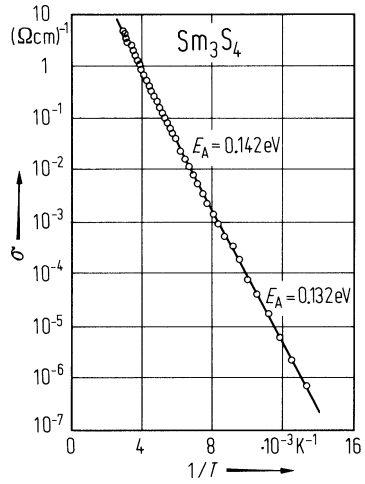
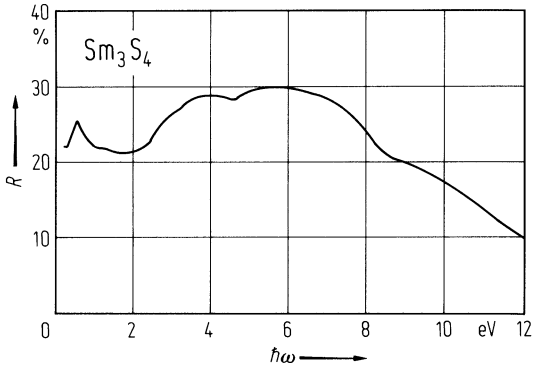


**Fig. 5.**

$Sm_3S_4$. Reflectivity vs. photon energy for single crystals at 300 K [76B1].



## Fig. 6.

$Sm_3S_4$. Electronic Raman scattering (relative intensity vs. Raman shift) at 4.2 K with 514.5 nm laser excitation. The peaks at 255 $cm^{-1}$ and 760 $cm^{-1}$ are assigned to the $^7F_0$–$^7F_1$ and $^7F_0$–$^7F_2$ transition of $Sm^{2+}$, respectively [77V].