substance: MoS_2
property: crystal structure, physical properties

2H-MoS_2

(S: structure (space group), CG: crystal growth, C: colour).

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

lattice parameters, resistivity, electron concentration

a	3.16 Å		S: hexagonal, D_{4h}^6 – $P6_3/mmc$	60J,
c	12.29 Å		CG: from polycrystalline mass at 1015°C	69C, 69W,
			C: black	72A,
$\rho_\perp$	33 Ω cm	n-type,	$d\sigma_\perp/dp$ = 0.065 Ω^{-1} cm^{-1}/kbar,	76N,
n	$6 \cdot 10^{15}$ cm^{-3}	synthetic	p < 10 kbar,	77E,
		single	$d\sigma_\perp/dp$ = 0.03 Ω^{-1} cm^{-1}/kbar,	78B,
		crystal	$12 \le p \le 30$kbar,	78E
			$\sigma_\perp/\sigma_\parallel \approx 200$.	
			($\rho_\perp$ = 0.27 Ω cm [70W].)	

energy gap

E_g	1.971 eV	T = 77 K	optical gap, dE_g/dp = – 3.8 meV/kbar (= – 2.5 meV/kbar for a natural crystal)
	0.7 eV		indirect gap, calculated
	1.4 eV		direct gap, calculated
$E_{g,th}$	0.47 eV	T < 300 K	
	1.27 eV	T > 790 K	

3R-MoS_2

(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)).

lattice parameters, resistivity, enery gap

a	3.17 Å		S: trigonal, C_{3v}^5 – R3m	67F,
c	18.38 Å		CG: halogen transport (947/890)	69C,
$\rho_\perp$	0.3 Ω cm	synthetic	$\sigma_\perp/\sigma_\parallel \approx 200$	70W,
E_g	1.9 eV	single	optical gap,	72A
$E_{g,th}$	0.25 eV	crystal	dE_g/dp = – 2.5 meV/kbar for a natural crystal	

MoS_2

(data for non-specified types)

resistivity, Hall mobility, electron concentration

$\rho_\perp$	18 Ω cm	n-type,	75G
$\mu_{H\perp}$	57 $cm^2/V\ s$	natural	
n	$6 \cdot 10^{15}\ cm^{-3}$	crystal	

energy gap

E_g	1.9 eV	optical gap
$E_{g,th}$	1.6 eV	

resistivity, Hall mobility, hole concentration

$\rho_\perp$	2.0 Ω cm	p-type,
$\mu_{H\perp}$	20 $cm^2/V\ s$	synthetic
p	$1.6 \cdot 10^{17}\ cm^{-3}$	single crystal

Figures to this document:

band structure: Fig. 1

Brillouin zone: Fig. 2b

electrical conductivity: Fig. 3

carrier concentration: Fig. 4

References:

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Fig. 1.

MoS_2. Band structure and density of states of 2H modification [78B].

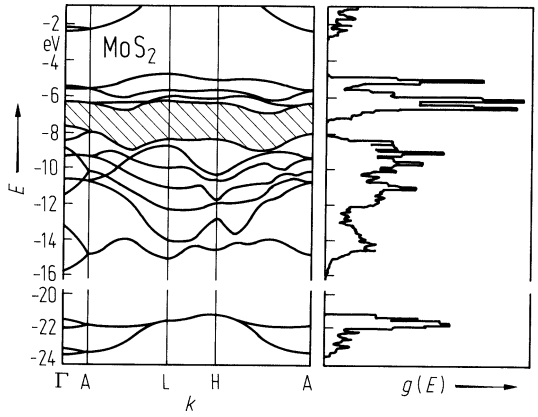

Fig. 2.

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

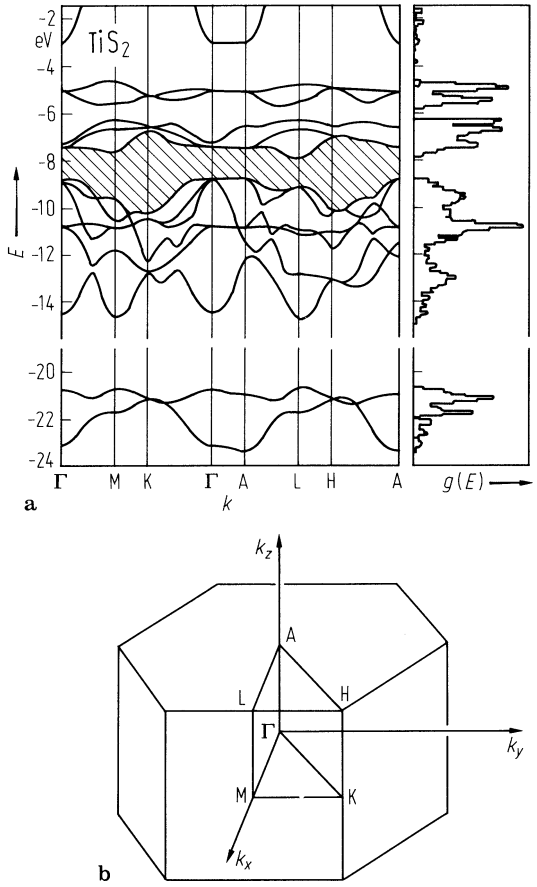

Fig. 3.

MoS_2. In plane electrical conductivity vs. pressure in 2H-MoS_2 at room temperature [78E]. σ in Ω^{-1} cm^{-1}.

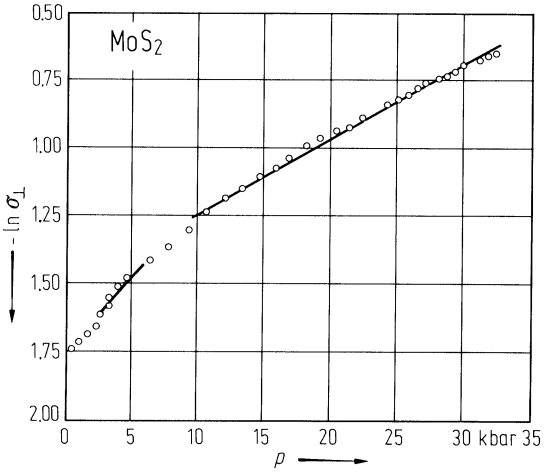

Fig. 4.

MoS_2, $MoSe_2$, WSe_2. Carrier concentration (in cm^{-3}) vs. reciprocal temperature for (a) three different single crystal samples of n-type 2H–MoS_2, (b) three different single crystal samples of n-type 2H– $MoSe_2$, (c) three different single crystal samples of p-type 2H–WSe_2. A line of representative slope is shown. Unless otherwise marked, the experimental errors are within the symbol representing each measurement [77E].