substance: NiS_2
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).

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

lattice parameters

a	5.69 Å		S: pyrite, C2, T_h^6 – Pa3	68B2,

resistivity, Seebeck coefficient, energy gap

ρ	1 Ω cm	p-type	CG: halogen transport (740/710)	68B3,
S	311 μV K^{-1}	synthetic single crystal	C: shiny black	70H,
E_g	0.27 eV		optical gap	71L,
$E_{g,th}$	0.64 eV	$T > 380$ K	Semiconductor-metal transition	71W,
	0.14 eV	$T = 140...380$ K	for $p > 30$ kbar at RT.	72G,
	0.009 eV	$T < 140$ K	$dT_{tr}/dp = 6(1)$ K/kbar	72K,
dE_g/dT	– 0.4 meV/K		E_g: optical gap	73G,
dE_A/dp	– 4.3(3) meV/kbar		$(= (1/2)(dE_{g,th}/dp)$	73M,

Néel and Curie temperatures

dT_N/dp	0.9(1) K/kbar		antiferromagnetic, $T_N \approx 50$ K, weak	75M,
dT_C/dp	0.4(1) K/kbar		ferromagnetism below $T_C = 30$ K,	77M,
			see text in document	78K,
				78M

Figures to this document:

lattice parameters: Fig. 1

resistivity: Figs. 2, 3

semiconductor-metal transition: Fig. 4

magnetization: Figs. 5, 10

electrical conductivity: Fig. 6

energy gap: Fig. 7

magnetic structure: Figs. 8, 9

density-of-states: Fig. 11

References:

68B1 Bertaut, E. F., Cohen, J., Lambert-Andron, H., Mollard, P.: J. Phys. (Paris) 29 (1968) 813.

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72K Kautz, R. L., Dresselhaus, M. S., Adler, D., Linz, A.: Phys. Rev. B6 (1972) 2078.

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78K Kikuchi, K., Miyadai, T., Fukui, T., Ito, H., Takizawa, K.: J. Phys. Soc. Jpn. 44 (1978) 410.

78M Mori, N., Watanabe, T.: Solid State Commun. 27 (1978) 567.

Fig. 1.

$NiS_{2\pm x}$. Lattice parameters at RT vs. stoichiometry (stoichiometry modified according to [73G]) [72G].

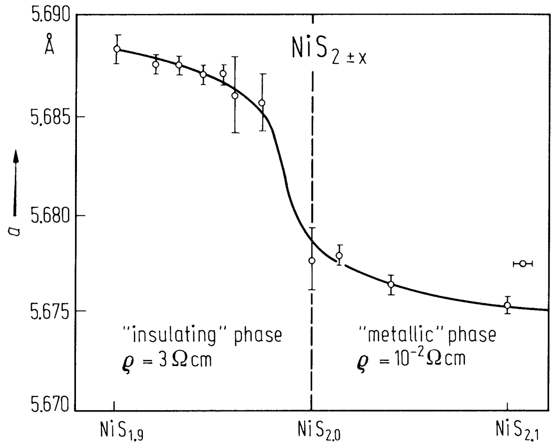

Fig. 2.

NiS_2. Resistivity vs. reciprocal temperature for a sample prepared under high pressure [68B1].

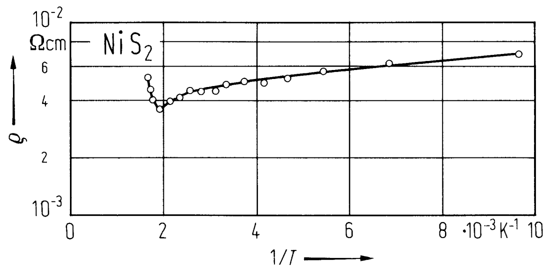

Fig. 3.

NiS_2. Resistivity vs. pressure at different temperatures for a single crystal [71W].

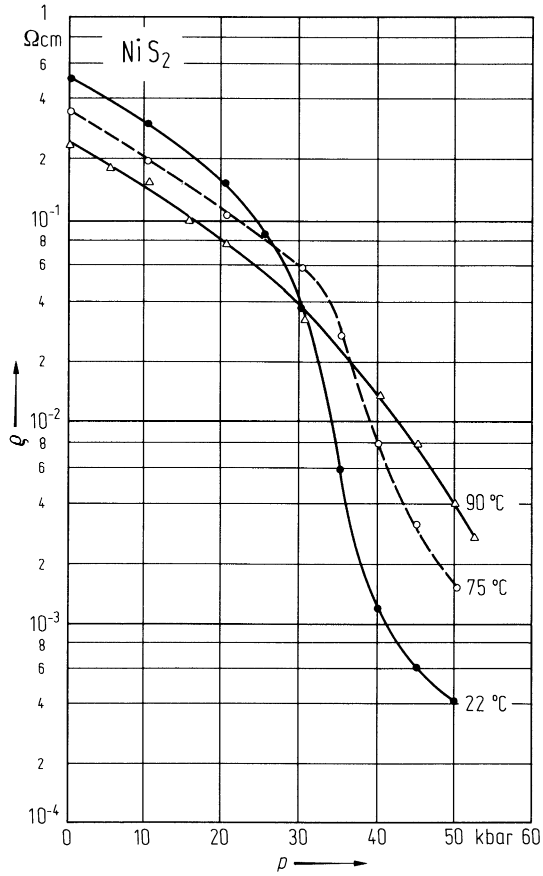

Fig. 4.

NiS_2. Semiconductor-metal transition boundary in a temperature-pressure diagram. The critical point predicted by this resistance measurement is shown by an arrow [73M].

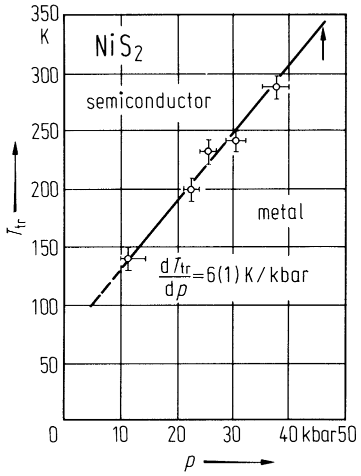

Fig. 5.

NiS_x. (a) Variation of the saturation magnetization σ_s and the number of nickel and sulfur vacancies, with nominal and experimental x, (b) positions of the resistivity and susceptibility maxima against experimental x [73G].

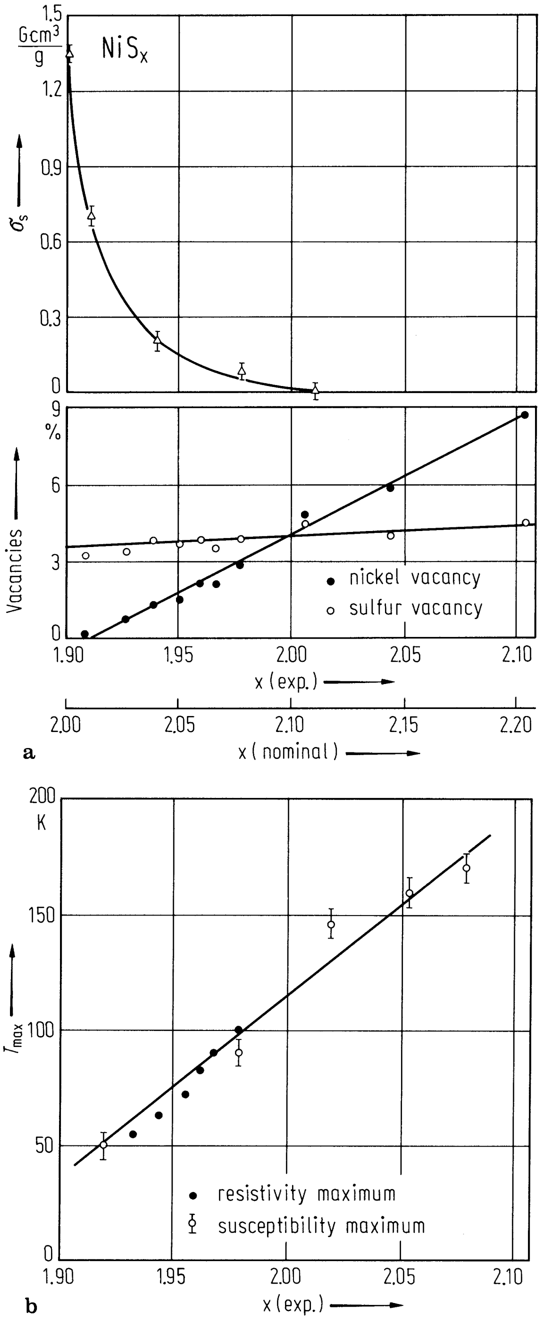

Fig. 6.

$NiS_{1.99}$. Electrical conductivity vs. inverse temperature between 100 and 610 K [72K].

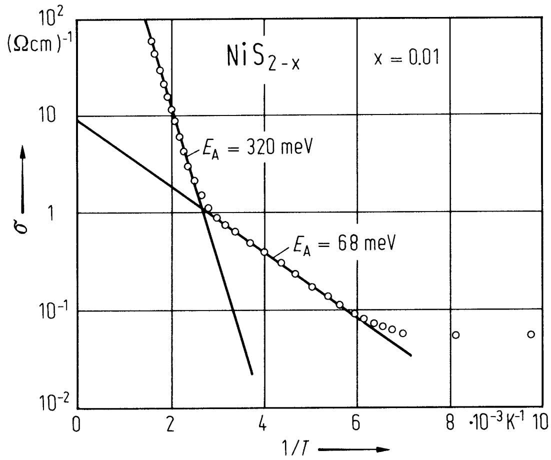

Fig. 7.

$NiS_{1.99}$. Optical energy gap vs. temperature [72K].

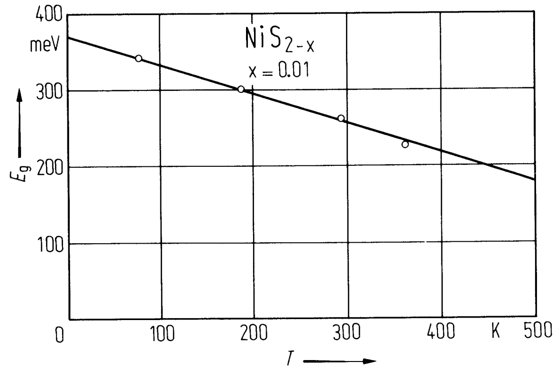

Fig. 8.

NiS_{2-x}. Magnetic sublattices for a general ordering of second kind of fcc lattice [78K]. Magnetic unit cells consist of 8 sublattices in which the spin directions of i and i'-th sites are antiparallel to each other.

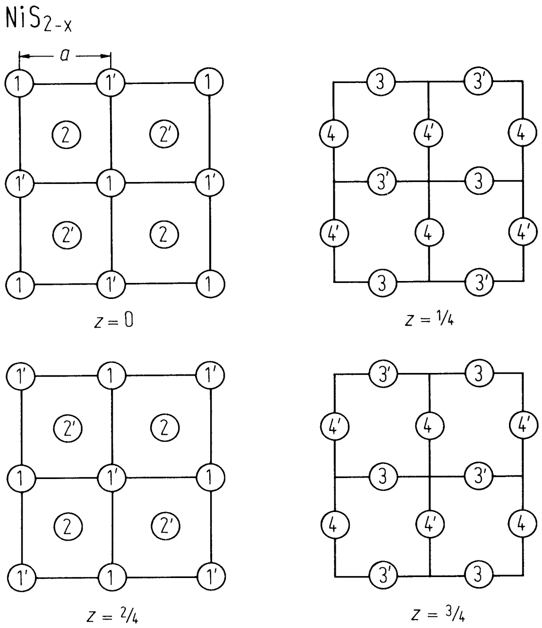

Fig. 9.

Projection of model-3 structure (Z_a-domain) onto four adjacent (001) planes. The solid or open circle denotes the positive or negative sign of *z* component of the spin, respectively. The direction cosines of each spin are S_1: ((-*a*)*bc*), $S_{1'}$: (*def*), S_2: ((-*a*)(-*b*)(-*c*)), $S_{2'}$: (*d*(-*e*)(-*f*)), S_3: (*ab*(-*c*)), $S_{3'}$: ((-*d*)*e*(-*f*)), S_4: (*a*(-*b*)*c*), $S_{4'}$: ((-*d*)(-*e*)*f*), with *a* = 0.04, *b* = 0.35, *c* = 0.94, *d* = 0.47, *e* = 0.87, *f* = 0.17 [78K].

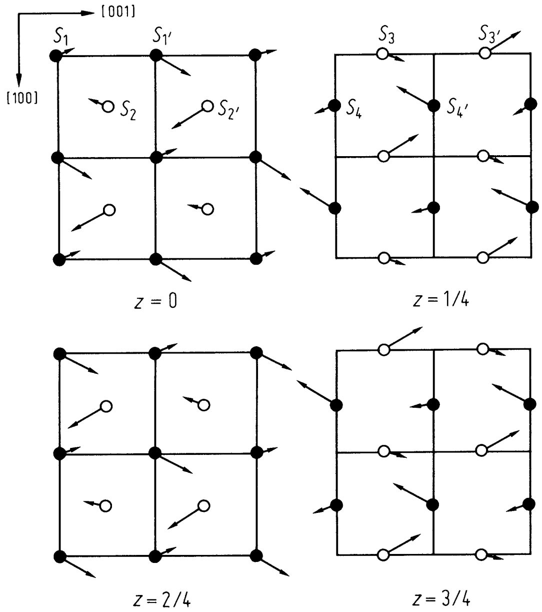

Fig. 10.

$NiS_{2\pm x}$. Spontaneous magnetization σ_0 vs. temperature [73G].

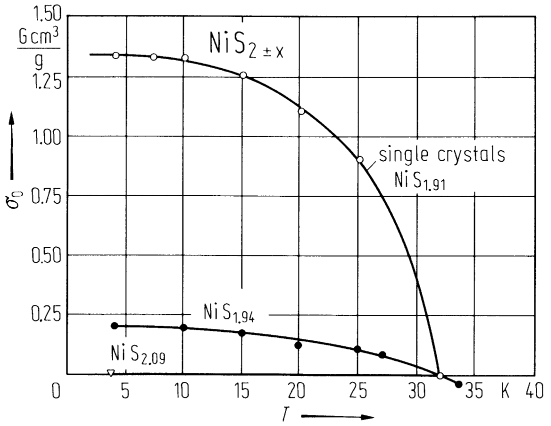

Fig. 11.

$NiS_{1.99}$. A density-of-states model. The electron occupation (shaded area) and various energies are given for T = 0 K. The upper impurity band is a donor band and the lower one an acceptor band [72K].