

substance: FeS₂

property: crystal structure, physical properties

FeS₂ (pyrite)

(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)).

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

lattice parameters

a	5.418 Å	S: pyrite, C2, T_h^6 – Pa3	54M, 68B1, 68B2, 76S, 79S, 83H
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density

d	5.0 g cm ⁻³	CG: chemical transport (715/655)
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resistivity, Seebeck coefficient, Hall mobility, Hall coefficient, energy gap

ρ	1.74 Ω cm	n-type
S	– 500 μV K ⁻¹	synthetic single
μ_H	230 cm ² /V s	crystal
R_H	– 400 cm ³ /C	
$E_{g,th}$	0.02 eV	$T < 60$ K
	0.4 eV	$T = 298$ K
	0.92 eV	$T = 500$ K

resistivity, Hall mobility, Hall coefficient, electron concentration, energy gap

ρ	0.06 Ω cm	n-type
μ_H	100 cm ² /V s	natural
R_H	– 6.5 cm ³ /C	crystal
n	$1.1 \cdot 10^{18}$ cm ⁻³	
E_g	0.95 eV	optical gap

resistivity, Hall mobility, Hall coefficient, hole concentration, energy gap

ρ	2.2 Ω cm	p-type
μ_H	1.3 cm ² /V s	natural
R_H	2.8 cm ³ /C	crystal
p	$2.6 \cdot 10^{18}$ cm ⁻³	
$E_g(T)$	$E_g(0) + aT + bT^2$	$T < 425$ K
		with $E_g(0) = 0.835$ eV, $a = 4 \cdot 10^{-5}$ eV/K $b = -7.4 \cdot 10^{-7}$ eV/K ²

FeS₂ (marcasite)

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

lattice parameters

<i>a</i>	4.44 Å	S: marcasite, C18, D _{2h} ¹² – Pnnm	70B1,
<i>b</i>	5.42 Å	CG: difficult to grow single	70B2,
<i>c</i>	3.39 Å	crystals, natural crystal available	83H

density

<i>d</i>	4.87 g cm ⁻³
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Figures to this document:

resistivity: Fig. 1

References:

- 54M Marinace, J. C.: Phys. Rev. 96 (1954) 593.
- 68B1 Bertaut, E. F., Cohen, J., Lambert-Andron, H., Mollard, P.: J. Phys. (Paris) 29 (1968) 813.
- 68B2 Bither, T. A., Bouchard, R. J., Cloud, W. H., Donohue, P. C., Siemons, W. J.: Inorg. Chem. 7 (1968) 2208.
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- 70B2 Brostigen, G., Kjekshus, A.: Acta Chem. Scand. 24 (1970) 2993.
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Fig. 1.

FeS₂ (pyrite). Resistivity vs. reciprocal temperature [68B1].

