TEMPERATURE REORIENTATION OF THE SPINS IN NATURAL PYRRHOTINE $Fe_{0.88}S$

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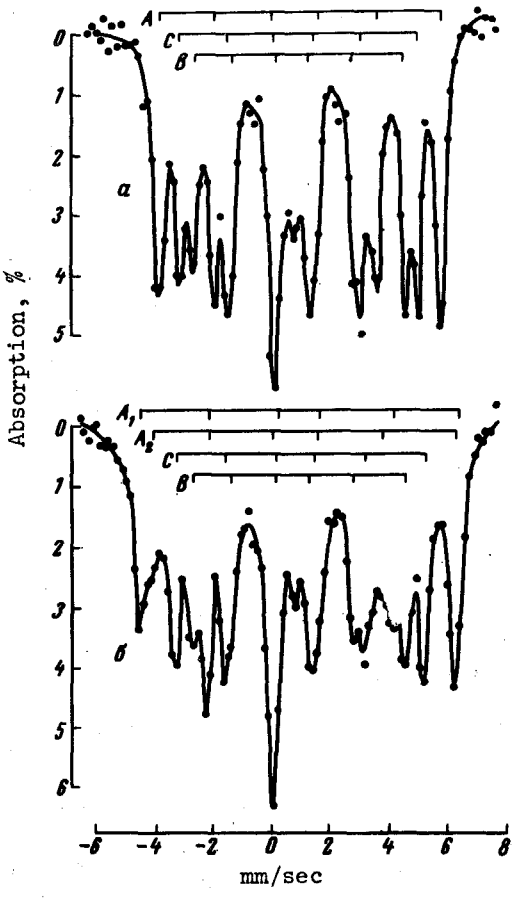
Investigations of the magnetic properties of pyrrhotine Fe_7S_8 ($Fe_{0.875}S$) have shown [1] that this crystal has a pseudohexagonal structure with a small monoclinic distortion, and has ferromagnetic properties as the result of the ordering of the vacancies. The magnetic moments of the iron ions are arranged antiparallel in alternating layers of cations, and lie in the basal plane at $T \sim 250°K$ [1, 2].

Magnetic measurements carried out in a wide temperature interval have shown [3, 4] that lowering the system temperature changes the iron-ion spin orientation relative to the crystallographic axes. We have investigated this phenomenon by nuclear γ resonance, and were thus able to trace the behavior of each of the three sublattices contained in $Fe_{0.880}S$. An essentially new result is that the spins in one of the sublattices become independently reoriented while the hyperfine-structure parameters in the other two remain constant.

The γ-resonance spectrum of $Fe_{0.88}S$ at $T = 300°K$ (Fig. a) is a superposition of three components of the magnetic-hyperfine structure of Fe^{57}. These components correspond to magnetically-nonequivalent positions of the iron [5, 6]. If only indirect exchange couplings are taken into account [6], the iron ions located in the A positions have no vacancies in the positions of the nearest neighbors, and are coupled by twelve exchange couplings with the oppositely oriented sublattices B and C. The cations in the B and C positions have respectively four and two vacancies in their immediate vicinity, and are characterized by ten and eight such couplings. Thus, the A cations on the one hand, and the B and C cations on the other, form a sequence of ferromagnetic planes (parallel to the basal plane) with mutually antiparallel spin directions. The cation distribution in Fe_7S_8 is given by

$$[\square Fe_3(A)][Fe_2(B)Fe_2(C)]S_8 .$$

As shown by an analysis of the γ-resonance spectra (figure), a splitting of the A components into two components A_1 and A_2 with quadrupole shifts $\Delta(A_1)$ and $\Delta(A_2)$ that have opposite signs and increase continuously in absolute magnitude up to the final measurement temperature $T = 88°K$, is observed starting with $T \sim 250°K$ (Fig. b).



γ-resonance spectra of $Fe_{0.88}S$ at 300°K (a) and 88°K (b). The positions of the hyperfine structure components are marked separately.

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The quadrupole shifts of the B and C components of the hyperfine structure remain practically unchanged. The characteristics of the spectra of $Fe_{0.88}S$ (Figs. a and b) are listed in the table. We note that the values of the hyperfine fields $H(A_1)$ and $H(A_2)$ in the two sublattices (T = 88°K) are different, probably because of the dipole contribution made to the hyperfine fields; this contribution is proportional to the electric field gradient in the region of the nucleus [7].

The temperature variations of the quadrupole shifts and of the values of the fields $H(A_1)$ and $H(A_2)$ show that the spin direction of the A sublattice is not collinear with the basal plane. At least two A-sublattices are produced, characterized by different angles θ_1 and θ_2 of the electronic magnetic moments of the ions relative to the hexagonal axis of the crystal. At the same time, the ion spins in the B and C sublattices obviously remain in the basal plane. A quantitative determination of the θ_1 and θ_2 is unfortunately difficult, since the tensor of the electric field gradient at the $Fe^{57}(A)$ nuclei is in this case not axially symmetrical ($V_{xx} \neq V_{yy}$), and the direction of the hyperfine field H(A) does not coincide with one of its principal axes [5, 8].

We have thus observed in this experiment in ordered $Fe_{0.88}S$ a continuous variation (in the temperature interval 250 - 88°K) of the orientation of the ion moments in the A-sublattice, i.e., in the sublattice not subject to the action of vacancies[2].

Parameters of hyperfine structure of γ resonance spectra of $Fe_{0.88}S$ at 300 and 88°K

T, °K	Hfs structure comp.	Relative intensity I_i	H_i, kOe	δ_i, mm/sec	Δ_i, mm/sec
300	A	1,34 ± 0,1	301 ± 3	+ 0,55 ± 0,01	+ 0,31 ± 0,03
	B	1,00 ± 0,1	224 ± 3	+ 0,53 ± 0,02	+ 0,43 ± 0,04
	C	1,02 ± 0,1	253 ± 4	+ 0,52 ± 0,02	+ 0,31 ± 0,04
88	A_1	0,83 ± 0,1	337 ± 3	+ 0,83 ± 0,02	− 0,11 ± 0,03
	A_2	0,52 ± 0,2	315 ± 5	+ 0,80 ± 0,03	+ 0,68 ± 0,06
	B	1,00 ± 0,1	225 ± 3	+ 0,77 ± 0,02	+ 0,41 ± 0,04
	C	1,04 ± 0,1	265 ± 3	+ 0,78 ± 0,02	+ 0,31 ± 0,04

δ_i - isomer shift (relative to metallic iron);
Δ_i - quadrupole splitting;
I_i - relative intensity;
H_i - hyperfine field.

It is interesting to note that in the high-temperature phase of stoichiometric FeS, i.e., the one without vacant sites, a complete reorientation of the spins from the basal plane to the direction of the C axis takes place in the vicinity of 400°K [9]. The parameters of the Mossbauer sextuplet of FeS

[2] No crystallographic changes were observed in Fe_7S_8 in the interval 77 - 300°K [4].

are close to the parameters of the considered A component of the hyperstructure of $Fe_{0.88}S$ [5, 9].

The results of detailed investigations of this phenomenon in single-crystal Fe_7S_8 absorbers are being readied for publication.

[1] E. Bertout, Acta Crystallogr. 6, 557 (1953).
[2] F.K. Lotgering, Philips Res. Reports 11, 190 (1956).
[3] M. Bin and R. Pautenet, J. Appl. Phys. 34, 1161 (1963).
[4] K. Sato, J. Phys. Soc. Japan 21, 733 (1966).
[5] S. Hafner and M. Kalvius, Z. Krist. 123, 443 (1967).
[6] N.S. Ovanesyan, V.A. Trukhtanov, G.Yu. Odinets, G.V. Novikov, and L. Cser, Zh. Eksp. Teor. Fiz. 60, No. 6 (1971) [Sov. Phys.-JETP 33, No. 6 (1971)].
[7] J.J. van Loef, J. Appl. Phys. 39, 1258 (1968).
[8] W. Kundig, Nucl. Instr. and Meth. 48, 219 (1966).
[9] R.C. Thiel and C.B. van den Berg, Phys. Stat. Sol. 29, 837 (1968).

INFLUENCE OF TWINS ON THE MAGNETORESISTANCE OF Sb

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As is well known, in many crystals subjected to an external force, the lattice is shifted to a new position prior to the occurrence of the failure, and a mechanical twin is produced. The twin part of the crystal is a reflection of the crystal lattice relative to a certain plane called the twinning plane.

In this paper we attempt to clarify the influence of the twinning planes[1)] on the magnetoresistance of Sb at low temperatures. The measurements were made on a single crystal with a structure of high perfection (the dislocation density on the (111) plane, determined with the aid of etch pits, did not exceed 10^2 cm^{-2}), grown by drawing from the melt [1].

To produce mechanical twins, the sample was immersed in liquid nitrogen and its edge was broken off. As a result, the part of the sample adjacent to the fracture, was pierced by twins, the average distance between which was 1 mm. The width of each twin was $\lesssim 10^{-2}$ mm, and the system of twinning planes had Miller indices (110).

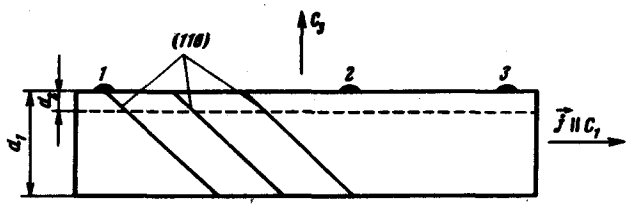

Fig. 1. Geometry of experiment: d_1 and d_2 - initial and final thickness of the sample; 1, 2, 3 - potential contacts; (110) - twinning plane (the thickness of the lines representing the twinning planes includes the twinning layers); $\vec{j}$ - electric-current vector.

The magnetoresistance of the "ideal" part of the crystal and the part containing the twins (we shall henceforth designate them

[1)] Here and throughout, when speaking of the influence of the twinning planes on the kinetic properties of Sb, we have in mind the real boundaries of the twins, and not ideal mathematical surfaces that have no thickness.