Noncollinear spin ordering in a hexagonal ferrite of type *W*

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A neutron-diffraction investigation of the spin ordering has been made in the hexagonal ferrite $BaNi_2Sc_2Fe_{14}O_{27}$ at temperatures 80 and 293 °K. The magnetic structure is an angular block structure; the angle between the spin axes of the blocks and the z axis is 55° at 80 °K and 43° at 293 °K. The projections of the magnetic moments on the basal plane in both cases constitute an antiphase ordering from block to block. The components of the block moments along the z axis are antiparallel at 80 °K and parallel at 293 °K. The Sc^{3+} ions are located at $2d$ ($z=0.25$) and $4f$ ($z=0.73$) sites. The Ni^{2+} ions are at octahedral $4f$ ($z=0.208$) sites.

In recent years a whole class of noncollinear spin orderings has been discovered in hexagonal ferromagnets; they have received the name "block" magnetic structures[1]. The essence of these orderings is that the well-known orientation arrangements (antiparallel, angular, spiral, etc.) of magnetic configurations are realized not by the magnetic moments of individual ions, but by the spin axes of groups of moments at boundaries of a part of the elementary cell (a block). The nature of the ordering of the magnetic axes of the blocks changes in a definite manner with the temperature and with applied magnetic fields. But the mutual orientation of the moments within a block meanwhile remains unchanged. The occurrence of such magnetic structures is due to peculiarities of the layered structure of hexagonal ferrimagnets and to a local order in the lattice of nonmagnetic ions, which weaken the exchange couplings between groups of magnetically active ions in the lattice of the ferrite.

The present article concerns the discovery of an angular block magnetic structure in a hexagonal ferrite of type **W**, which was known previously as a collinear ferrimagnet.

EXPERIMENTAL PART

A neutron-diffraction investigation of the spin ordering was made on a ferrite of type **W** with the chemical formula $BaNi_2Sc_2Fe_{14}O_{27}$ (Ni_2Sc_2W) at temperatures 80 and 293° K. This compound crystallizes in space group $P6_3/mmc$, with unit cell parameters $a=5.88$ Å and $c=32.8$ Å[2]. The specimens used were grain-oriented and had the form of a prism with dimensions $5\times5\times40$ mm. The axis of the texture was oriented along direction [001] and was normal to one of the faces of the prism.

A phase analysis of the specimens was carried out on an x-ray diffractometer URS-50IM. The x-ray photograph showed intense $00l$ lines, belonging to phase **W**. The intensities of the reflections of extraneous phases did not exceed 3% of the reflections of the basic phase of the ferrite under investigation.

Neutron-diffraction patterns were taken on the neutron-diffraction apparatus of the Institute of Solid-State Physics of the USSR Academy of Sciences. The wavelength of the neutrons used was 1.07 Å. The neutron-diffraction patterns were taken with motion of the detector and of the specimen in the ratio 2:1.

Figure 1a shows the neutron-diffraction pattern of a specimen of the ferrite under investigation at temperature 80° K ($00l$ reflections). Besides reflections $00l$ with even l, which are allowed by space group $P6_3/mmc$, there are observed on the pattern intense lines with odd l. Figure 1b shows the diffraction pattern of the same compound at 293° K. The diffraction lines filled in with black, $00l$ ($l=2n$), were obtained on a specimen heated above the Curie temperature (780° K). From a comparison of the patterns in Fig. 1 it follows that the $00l$ reflections with odd l are caused by magnetic scattering of the neutrons. Furthermore, at 293° K magnetic contributions are recorded both in the $00l$ reflections with even indexes l and in those with odd.

Figure 2a shows a model of the magnetic structure of the compound under investigation, obtained in the present research at 80° K. There is an antiparallel ordering of the magnetic axes $\mathbf{H_B}$ of the blocks B. In an elementary cell there are two blocks B with surfaces of separation between them, lying in a plane of mirror reflection. The angle between the spin axes of the blocks B and the z axis is 55°. The components of the magnetic axes of the blocks in the basal plane, $H_{B\perp}$, form an antiphase ordering from block to block; this is the reason for allowance of magnetic reflections with odd l. The ordering of the magnetic moments within a block is collinear, in agreement with the scheme proposed by Gorter[3].

Figure 2b shows the ordering scheme of the magnetic axes of the blocks in the ferrite under investiga-

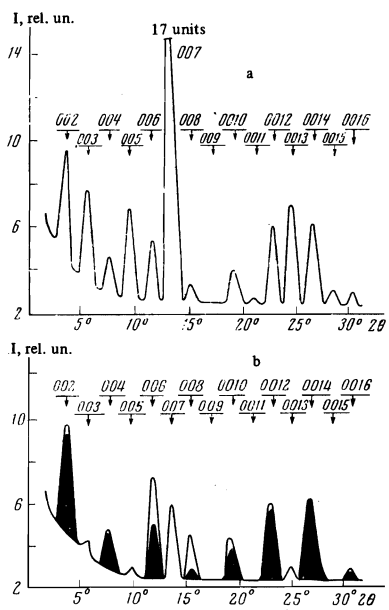

FIG. 1. Neutron diffraction patterns of the ferrite $BaNi_2Sc_2Fe_{14}O_{27}$: a, at 80°K; b, at 293° and 780°K.

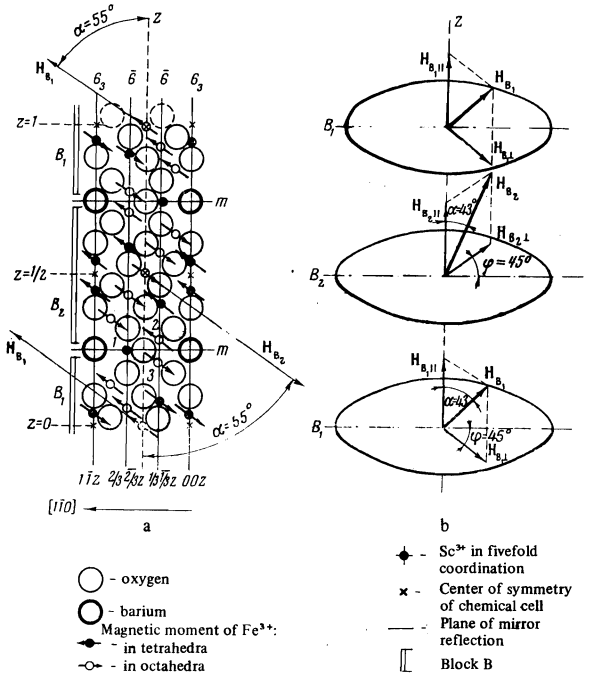

FIG. 2. Model of magnetic ordering of the ferrite investigated: a, magnetic structure at 80°K; b, ordering scheme of the magnetic axes of the blocks at 293°K. Here $H_{B\parallel}$ is the projection of the total magnetic moment vector on the z axis, and $H_{B\perp}$ is the projection of the total magnetic moment vector on the basal plane.

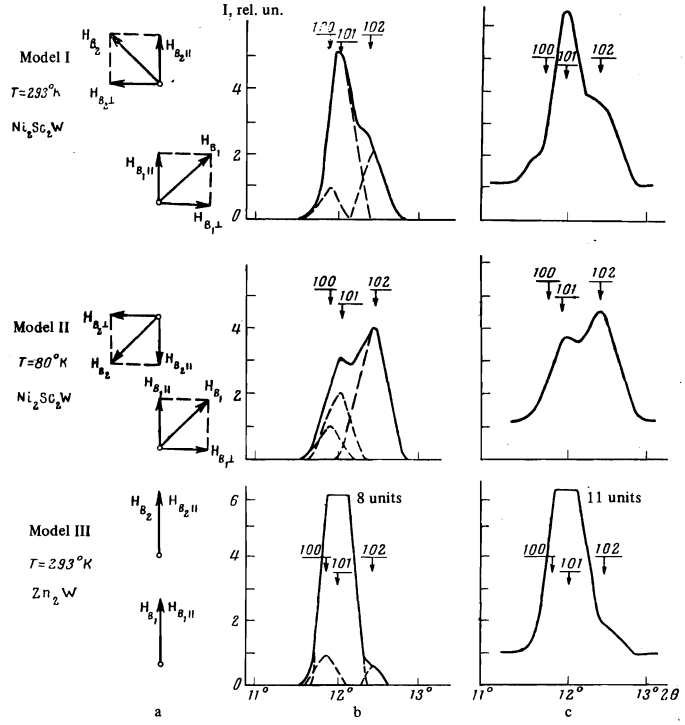

FIG. 3. Experimental and theoretical neutron-diffraction patterns from planes (100), (101), and (102) for ferrites Ni_2Sc_2W and Zn_2W. a, models of the mutual ordering of the total moments H_B of blocks B. b, theoretical patterns of neutron diffraction from planes (h0l); reflections 100, 101, and 102. c, experimental diffraction patterns; reflections 100, 101, and 102.

tion at 293° K. Here, in contrast to the structure at 80° K, the projections $H_{B1\perp}$ and $H_{B2\perp}$ of the magnetic moments of the blocks form an angular ordering with angle $\varphi = 90°$. At 293° K the angle between the spin axes of the blocks and the z axis is $\alpha = 43°$.

A comparison of calculated and measured values of the 00l reflection intensity, at 80° and 293° K, is given in the table. The uncertainty in the value of the angle between the spin axes of the blocks is ±5°.

From an analysis of the intensity of magnetic scattering of neutrons from (00l) planes it is not possible to draw a unique conclusion regarding the mutual ordering of the axis components $H_{B1\parallel}$ and $H_{B2\parallel}$. But since the magnetic configurations with parallel and antiparallel orientations of the components $H_{B\parallel}$ show up differently in reflections h0l, we carried out an analysis of the intensity of reflections 100–104 in order to determine the mutual ordering of the components $H_{B1\parallel}$ and $H_{B2\parallel}$.

Figure 3 shows calculated and experimental data on reflections h0l for three models with parallel and antiparallel ordering of the components $H_{B\parallel}$. As a specimen with collinear magnetic axis structure (model III), we used the hexagonal ferrite of type W of composition $BaZn_2Fe_{16}O_{27}$ (Zn_2W).

Comparison of the experimental and calculated data enabled us to conclude that in the ferrite Ni_2Sc_2W the components $H_{B1\parallel}$ and $H_{B2\parallel}$ are ordered antiparallel at 80° K and parallel at 293° K. It follows from our investigation that the Sc^{3+} ions are located at 2d (z = 0.25) and 4f (z = 0.073) positions. The most probable site for the Ni^{2+} ions is an octahedral 4f (z = 0.208) position.

In the calculations of the magnetic contributions to the reflections, the values of the magnetic form factors of the Fe^{3+} and Ni^{2+} ions were taken from the paper of Nathans et al.[4] The magnetic moments of the Fe^{3+} and

Measured and calculated values of intensities of reflections 00l of the ferrite investigated, at 80° and 293°K

00l	80° K		293° K		00l	80° K		293° K	
	I_{calc}	I_{exp}	I_{calc}	I_{exp}		I_{calc}	I_{exp}	I_{calc}	I_{exp}
002	250	250	242	260	0011	1	8	0	0
003	181	210	22	20	0012	176	180	180	170
004	80	78	76	90	0013	248	230	32	30
005	204	220	25	20	0014	250	218	265	210
006	118	136	252	230	0015	28	30	4	0
007	950	940	178	170	0016	12	10	10	10
008	36	30	80	84	0017	3	4	0	0
009	0	0	0	0	0018	1	0	0	0
0010	111	70	113	90	0019	6	4	3	0

Ni^{2+} ions were taken as 4.2 and 2.6 μ_B. In the calculations of the reflection intensity at 293° K, use was made of the mean value of the temperature factor B = 0.64 Å^2 given by Braun[2].

DISCUSSION OF RESULTS

According to the data of the present research, the noncollinear ordering observed in a ferrite of type W is due to a breaking of the exchange interaction between pairs of ions 1-2 and 1-3 (see Fig. 2a), caused by the arrangement of Sc^{3+} ions in 2d positions. Then, according to Koroleva and Mitina[5], the orientation of the magnetic moments in the blocks B_1 and B_2, which are separated by a mirror plane, can be influenced by the anisotropic superexchange interaction of Moriya[6]. This interaction is much weaker than the indirect exchange interaction. It can determine the magnetic ordering only when there is an appreciable weakening or breaking of the exchange couplings.

The energy of the Moriya superexchange interaction is written in the form $D \cdot S_1 \times S_2$, where D is the Moriya

interaction vector and where S_1 and S_2 are the spin vectors of the interacting ions. The superexchange interaction tends to unfold the vectors D, S_1, and S_2 at right angles to one another. According to Moriya's second rule [6], for a hexaferrite of type W the vector D is located in the basal plane. Consequently the magnetic axes of blocks B_1 and B_2 can be expected to have angular ordering with angle $\sphericalangle(\mathbf{H}_{B1}, \mathbf{H}_{B2}) \sim 90°$. Ordering of this sort was observed in the ferrite under investigation at 293° K. The appreciable increase of the angle between $\mathbf{H}_{B1}$ and $\mathbf{H}_{B2}$ upon lowering of the temperature to 80° K must apparently be due to a strengthening of the role of the indirect exchange interaction at the boundary between blocks.

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