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Monte Carlo simulation of spin-reorientation transition in weak ferrimagnets $YFeCrO_3$

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This work presents the modeling of the magnetic 3*d*-sublattice in mixed orthoferrites–orthochromites $YFe_{1-x}Cr_xO_3$ using classical Monte Carlo methods. It is shown that, when taking into account the competition of the Dzyaloshinskii vectors in the mixed compositions, magnetic moment compensations are observed, as well as angular magnetic configurations corresponding to the spin reorientation.

Keywords: weak ferrimagnetism, spin reorientation, negative magnetization, Dzyaloshinskii–Moriya interaction, Monte Carlo method, orthoferrites, orthochromites.

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1. Introduction

Systems based on orthoferrites-orthochromites of $RFe_{1-x}Cr_xO_3$ (R = Nd, Gd, Dy, Y, Lu) type were the subject of intense fundamental theoretical and experimental studies in the end of 20th century [1–9]. A new surge of interest in these systems already in the 21st century is associated with the finding of specific magnetoelectric and magnetocaloric properties [10–13] and the new prospects for practical application of the phenomena of temperature compensation of the magnetic moment, exchange bias and spin reorientation to create various multifunctional devices, for example, of spintronics [14–22].

The fundamental studies of orthoferrites and orthochromites are sill based first of all on the features of $4f-3d$-interaction and antisymmetric Dzyaloshinskii–Moriya (DM) exchange [1,23–27]. From the microscopic theory of antisymmetric exchange for the systems of $RFe_{1-x}Cr_xO_3$ type it is possible to obtain both the numerical estimation of the Dzyaloshinskii vector value and, what is especially important, its sign, which once played a principal role in the prediction and experimental discovery of a new type of magnetic ordering — weak ferrimagnetism [25]. The key feature of weak ferrimagnets is the competition of Dzyaloshinskii vectors between ion pairs $Fe^{3+}-Fe^{3+}$ and $Cr^{3+}-Cr^{3+}$ on the one hand and ion pairs $Fe^{3+}-Cr^{3+}$ and $Cr^{3+}-Fe^{3+}$ on the other hand.

Despite its long history, the unusual effect of the spontaneous spin reorientation (SR) in weak ferrimagnets with a non-magnetic R-ion (Y, Lu) in the absence of the external fields has not yet been described adequately. Usually the researchers limit themselves to phenomenological approaches and mean field approximations [1–3,25,28], using which, one can relate the possibility to change the Neel vector orientation $G_z \leftrightarrow G_x$ with microscopic nature of DM-interaction in the mixed orthoferrites-orthochromites $YFe_{1-x}Cr_xO_3$. The tools making it possible to „observe“ and study the magnetic configurations in these systems are Monte Carlo methods. These methods have already been used previously for modeling of rare-earth perovskites [29–33] and also mixed orthoferrites–orthochromites [34,35], but the authors have never considered the phenomena of spin reorientation.

Therefore, the main objective of the paper is development of the Monte Carlo (MC) method, which makes it possible to observe and study the complex magnetic configurations that are not typical for „parent“ $YFeO_3$ and $YCrO_3$ in the mixed orthoferrites–orthochromites $YFe_{1-x}Cr_xO_3$.

2. Model

Weak ferrimagnets of $YFe_{1-x}Cr_xO_3$ type are orthorhombic perovskites with the space group $Pbnm$. There are 4 magnetic 3*d*-ions per unit cell, for which the following classical basis vectors can be introduced [3]:

$$\begin{aligned} 4S\mathbf{F} &= \mathbf{S}^{(1)} + \mathbf{S}^{(2)} + \mathbf{S}^{(3)} + \mathbf{S}^{(4)}, \\ 4S\mathbf{G} &= \mathbf{S}^{(1)} - \mathbf{S}^{(2)} + \mathbf{S}^{(3)} - \mathbf{S}^{(4)}, \\ 4S\mathbf{C} &= \mathbf{S}^{(1)} + \mathbf{S}^{(2)} - \mathbf{S}^{(3)} - \mathbf{S}^{(4)}, \\ 4S\mathbf{A} &= \mathbf{S}^{(1)} - \mathbf{S}^{(2)} - \mathbf{S}^{(3)} + \mathbf{S}^{(4)}. \end{aligned} \quad (1)$$

Here the vector **G** describes the main antiferromagnetic component of the magnetic structure, **F** is the vector of weak ferromagnetism (overt canting of sublattices), weak antiferromagnetic components **C** and **A** describe the canting

of magnetic sublattices without formation of the total magnetic moment (hidden canting of sublattices). Typical spin configurations for the $3d$-sublattice, compatible with the antiferromagnetic sign of the main isotropic superexchange, are indicated as $\Gamma_1(A_x, G_y, C_z)$, $\Gamma_2(F_x, C_y, G_z)$, $\Gamma_4(G_x, A_y, F_z)$, where the brackets contain the only nonzero components of basis vectors.

Contrary to $YFeO_3$ and $YCrO_3$, which are weak ferromagnet with the main magnetic structure of $\Gamma_4(G_x, A_y, F_z)$ type below Neel temperature T_N, weak ferrimagnets orthoferrites–orthochromites $YFe_{1-x}Cr_xO_3$ according to the data of magnetic measurements show full or partial spin-reorientation of $G_xF_z-G_zF_x$ type in the wide range of substitution [2]. Usually in such systems the reorientation arises due to $4f-3d$-interaction [3], but in case of non-magnetic yttrium ion such mechanism is excluded, and anisotropy of $3d$-sublattice must be considered. And indeed, the phenomenon can be explained by the strong reduction in the contribution of DM-interaction into the magnetic anisotropy [7,28].

Let us present the spin-Hamiltonian of a weak ferrimagnet in the simplest form, taking into account only the contributions of the isotropic exchange interaction, and also the antisymmetric Dzyaloshinskii–Moriya exchange:

$$\hat{H} = \hat{H}_{ex} + \hat{H}_{\mathrm{DM}}$$

$$\hat{H}_{ex} = \frac{1}{2}\sum_{\langle ij\rangle} I_{ij}(\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j),$$

$$\hat{H}_{\mathrm{DM}} = \frac{1}{2}\sum_{\langle ij\rangle} \mathbf{d}_{ij}[\hat{\mathbf{S}}_i \times \hat{\mathbf{S}}_j] \qquad (2)$$

summation runs over nearest neighbors, I_{ij} is the exchange integral, $\mathbf{d}_{ij}$ the Dzyaloshinskii vector.

Figire 1 shows the structure of superexchange bonds in the model. The cation-anion distances and the superexchange bond angles for the nearest neighbors slightly differ, so below we assume the equality of the superexchange integrals $I_{ab} = I_c = I$ and the modules of the Dzyaloshinskii vectors $d_{ab} = d_c = d$, although the vectors themselves are directed in different directions. Let us also presume further that the pairs of nearest ions lie along the axes of the system of coordinates $x'y'z'$, which is rotated around axis z by angle 45°; however, all vector values in the paper are calculated in the system xyz, axes of which correspond to the crystal abc axes.

Microscopic expression of the relation between Dzyaloshinskii vector and the geometry of the superexchange cation–anion–cation bond is as follows [1]

$$\mathbf{d}_{ij} = d_{ij}(\theta)[\mathbf{r}_i \times \mathbf{r}_j], \qquad (3)$$

where $\mathbf{r}_{ij}$ are unit vectors along bonds $O^{2-}-Fe^{3+}$, or $O^{2-}-Cr^{3+}$, θ the angle of superexchange bond (hereinafter it will be omitted in the designations). The structure factors determining the orientation of the Dzyaloshinskii vectors in orthoferrites–orthochromites of the $YFe_{1-x}Cr_xO_3$ are given

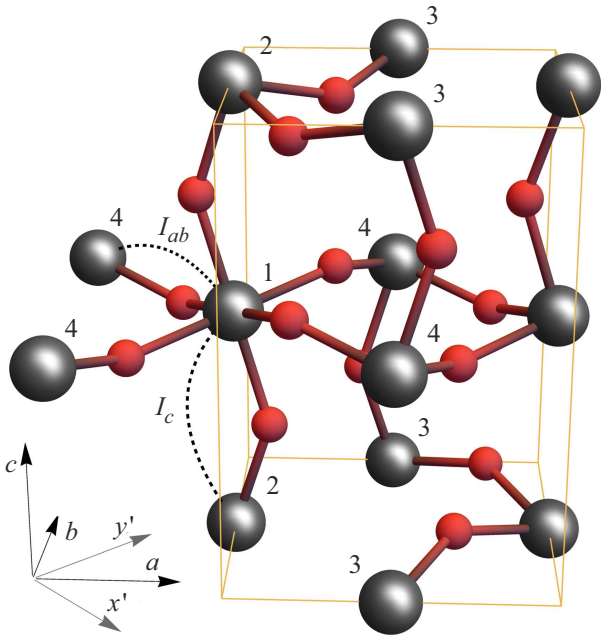

Figure 1. The structure of superexchange bonds; large balls are Fe^{3+}, Cr^{3+} ions, small balls are O^{2-}; *1, 2, 3, 4* are magnetic ions in four non-equivalent positions.

in the table. The simple formula (3) allows determining a direct relationship of magnetic non-collinearity (overt and hidden canting of sublattices) in weak ferromagnets with the crystal structure [23–25].

In accordance with the crystal symmetry, the clear view of the Dzyaloshinskii vectors depending on the site number is as follows:

$$\mathbf{d}_{ijk}(Ox') = d\begin{pmatrix}(-1)^{i+j+k}\alpha_{ab}\\(-1)^{i+j+k}\beta_{ab}\\(-1)^{i+j}\gamma_{ab}\end{pmatrix} \qquad (4)$$

$$\mathbf{d}_{ijk}(Oy') = d\begin{pmatrix}-(-1)^{i+j+k}\alpha_{ab}\\(-1)^{i+j+k}\beta_{ab}\\(-1)^{i+j}\gamma_{ab}\end{pmatrix} \qquad (5)$$

$$\mathbf{d}_{ijk}(Oz') = d\begin{pmatrix}(-1)^{k}\alpha_{c}\\(-1)^{i+j+k}\beta_{c}\\0\end{pmatrix}, \qquad (6)$$

where index i numbers ions along axis x', j along axis y', k along axis z', $\mathbf{d}_{ijk}(Ox')$ is vector for pairs of ions, on the

Components x, y, z of structure factors $[\mathbf{r}_i \times \mathbf{r}_j]$ calculated using the neutron diffraction data [11] for $YFe_{0.5}Cr_{0.5}O_3$

	x	y	z
$[\mathbf{r}_2 \times \mathbf{r}_1]$	$\alpha_c = 0.216$	$\beta_c = 0.562$	0
$[\mathbf{r}_4 \times \mathbf{r}_1]$	$\pm\alpha_{ab} = 0.303$	$\beta_{ab} = 0.287$	$\gamma_{ab} = 0.397$

site ijk and its nearest neighbor along axis x', $\mathbf{d}_{ijk}(Oy')$ — vector for ion pairs along axis y', $\mathbf{d}_{ijk}(Oz')$ — vector for ion pairs along axis z'.

3. Methods

For numerical modeling of a simple cubic $3d$-lattice with Hamiltonian (2) we considered the two Monte Carlo (MC) methods with the different methods of state selection in the lattice site within the Metropolis algorithm [36].

In the first case it is a pure classical Monte Carlo method (MC1), when spin operators $\hat{\mathbf{S}}_i$ in the Hamiltonian (2) are substituted with the classical vectors

$$\mathbf{m}_i = S_i \begin{pmatrix} \cos v_i \sqrt{1-u_i^2} \\ \sin v_i \sqrt{1-u_i^2} \\ u_i \end{pmatrix}, \tag{7}$$

where u_i is a random value from -1 to $+1$, v_i is a random value from 0 to 2π, S_i is the spin quantum number of the corresponding site. This is one of the simplest MC methods, which is often used in the work with the spin-Hamiltonian of type (2), including for description of magnetic phenomena in rare-earth perovskites [29,30,32,35,37].

At the initial step of MC, at each site of the lattice i, the numbers $u_i^{(0)}$, $v_i^{(0)}$ are selected randomly, the magnetic moments $\mathbf{m}_i$ and system energy $E^{(0)}$ are calculated. At the next step the new random numbers $u_i^{(1)}$, $v_i^{(1)}$ are selected, and also between 0 and 1 the random number p is selected, then the corresponding energy and its change are calculated relative to the previous state of the system $\Delta E = E^{(1)} - E^{(0)}$. If the new state complies with the inequation $\exp(-\Delta E/T) > p$, where T is the system temperature, we accept the new state of the system: $u_i^{(0)} \to u_i^{(1)}$, $v_i^{(0)} \to v_i^{(1)}$, if the new state does not comply with the inequation, we leave the previous state of the system. This step is repeated until the system reaches equilibrium at the specified temperature T.

In the second case we propose the quasi-classical Monte Carlo (MC2) method, when the site state is specified by the wave function $|\psi\rangle = \sum_M c_M |S, M\rangle$, where S is the site spin, M is the spin projection on the axis, c_M are random coefficients with normalization $\langle\psi|\psi\rangle = 1$ (site indices are omitted).

In case of the iron ions (spin $S = 5/2$) the wave function has the following form

$$|\psi\rangle = c_{-\frac{5}{2}}\left|\frac{5}{2}, -\frac{5}{2}\right\rangle + c_{-\frac{3}{2}}\left|\frac{5}{2}, -\frac{3}{2}\right\rangle + c_{-\frac{1}{2}}\left|\frac{5}{2}, -\frac{1}{2}\right\rangle + c_{\frac{1}{2}}\left|\frac{5}{2}, \frac{1}{2}\right\rangle + c_{\frac{3}{2}}\left|\frac{5}{2}, \frac{3}{2}\right\rangle + c_{\frac{5}{2}}\left|\frac{5}{2}, \frac{5}{2}\right\rangle, \tag{8}$$

with coefficients presented as

$$c_{\frac{5}{2}} = \sqrt{1-\xi_1^{\frac{1}{5}}}\, e^{i2\pi\xi_{\frac{5}{2}}},$$

$$c_{\frac{3}{2}} = \xi_1^{\frac{1}{10}}\xi_2^{\frac{1}{8}}\xi_3^{\frac{1}{6}}\xi_4^{\frac{1}{4}}\xi_5^{\frac{1}{2}}\, e^{i2\pi\xi_{\frac{3}{2}}},$$

$$c_{\frac{1}{2}} = \xi_1^{\frac{1}{10}}\xi_2^{\frac{1}{8}}\sqrt{1-\xi_3^{\frac{1}{3}}}\, e^{i2\pi\xi_{\frac{1}{2}}},$$

$$c_{-\frac{1}{2}} = \xi_1^{\frac{1}{10}}\xi_2^{\frac{1}{8}}\xi_3^{\frac{1}{6}}\sqrt{1-\xi_4^{\frac{1}{2}}}\, e^{i2\pi\xi_{-\frac{1}{2}}},$$

$$c_{-\frac{3}{2}} = \xi_1^{\frac{1}{10}}\xi_2^{\frac{1}{8}}\xi_3^{\frac{1}{6}}\xi_4^{\frac{1}{4}}\sqrt{1-\xi_5}\, e^{i2\pi\xi_{-\frac{3}{2}}},$$

$$c_{-\frac{5}{2}} = \xi_1^{\frac{1}{10}}\sqrt{1-\xi_2^{\frac{1}{4}}}\, e^{i2\pi\xi_{-\frac{5}{2}}}, \tag{9}$$

where all ξ_q, ξ_M are random values from 0 to 1. In case of chromium ions with spin $S = 3/2$, it is necessary to set $\xi_1 = \xi_2 = 1$. Such parameterization of the coefficients guarantees the normalization of the wave function on the site and that any state with the uniform sampling ξ_q, ξ_M will appear with the same frequency in the algorithm operation.

Therefore, in the MC2 method the magnetic moment per site and the system energy are accordingly calculated as

$$\mathbf{m}_i = \langle\psi_i|\hat{\mathbf{S}}_i|\psi_i\rangle, \tag{10}$$

$$E = \langle\Psi|\hat{H}|\Psi\rangle, \tag{11}$$

where $|\Psi\rangle = \Pi_i|\psi_i\rangle$ is the wave function of the entire system. This method works using the same Metropolis algorithm as the one given above for MC1, but using formulas (8)–(11).

For the characterization of the angular phase, at each step of MC (after achievement of equilibrium in the system) both methods calculate the basis vectors (1) in the entire lattice as

$$F = \frac{1}{N}\sum_{ijk}^{N}\frac{\mathbf{m}_{ijk}}{S_{ijk}}, \quad G = \frac{1}{N}\sum_{ijk}^{N}(-1)^{i+j+k}\frac{\mathbf{m}_{ijk}}{S_{ijk}},$$

$$C = \frac{1}{N}\sum_{ijk}^{N}(-1)^{i+j}\frac{\mathbf{m}_{ijk}}{S_{ijk}}, \quad A = \frac{1}{N}\sum_{ijk}^{N}(-1)^{k}\frac{\mathbf{m}_{ijk}}{S_{ijk}}, \tag{12}$$

where index i numbers ions along axis x', j along axis y', k along axis z', N is the number of $3d$-ions, S_{ijk} is the spin of site ijk, $\mathbf{m}_{ijk}$ is the magnetic moment of site ijk, calculated using formula (7) in MC1 method and formula (10) in MC2 method.

4. Results

Numerical simulation was carried out using a simple cubic lattice of $N = 64 \times 64 \times 64$ sites with periodic boundary conditions. In accordance with concentration x each site is randomly selected as an iron or a chromium ion. To establish the equilibrium, at the specified values of temperature and concentration, $2 \cdot 10^4$ MC steps were made at each site of the lattice, and then another $3 \cdot 10^4$ MC steps to the site for statistics collection.

Based on the results in the mean field approximation (MFA) [28], the Hamiltonian parameters in this paper take the following values: $I_{\mathrm{FeFe}} = 36.6\,\mathrm{K}$, $I_{\mathrm{CrCr}} = 18.7\,\mathrm{K}$,

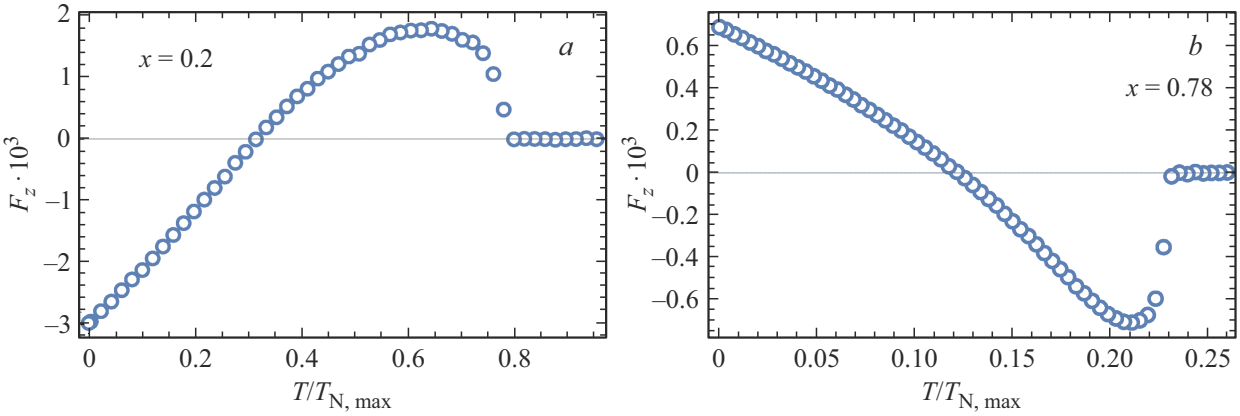

Figure 2. The first (a) and second (b) compensations of weak ferromagnetic vector **F** in MC1 method.

$I_{FeCr} = 13.4$ K, $d_{FeFe} = 2.0$ K, $d_{CrCr} = 1.7$ K, $d_{FeCr} = -2.5$ K, where the negative sign of the parameter d_{FeCr}, relative to d_{FeFe} and d_{CrCr}, specifies in the model system the competition of Dzyaloshinskii vectors.

Note at once that the considered systems of $N = 64^3$ ions are far from the size of the real samples, and the results may depend on how the impurity will be distributed at specific modeling. For example, with the considerable quantity of impurity ($x \approx 0.5$) the system will contain different areas: when all nearest neighbors of the selected ion are ions of the same type (where the contribution is provided only by vectors $\mathbf{d}_{FeFe}$ and $\mathbf{d}_{CrCr}$), and when all closest neighbors are ions of another type (where the contribution is provided only by vector $\mathbf{d}_{FeCr}$), and depending on the relative volume of the areas, the value and the direction of basis vectors (1) will differ. In this paper we will not study the possible effects.

The calculations using the MC1 method show that in the mixed orthoferrite–orthochromite $YFe_{1-x}Cr_xO_3$ below the critical temperature $T_N(x)$ a spontaneous transition occurs from a disordered state into a phase with the single non-zero components of basis vectors $G_x, A_y.F_z$, i. e. into phase Γ_4. In this context the MC1 method agrees with MFA, including a conclusion that for reorientation into the phase different from $\Gamma_4(G_x, A_y, F_z)$, single competition of Dzyaloshinskii vectors is not sufficient and, for example, it is necessary to take into account the effects of the single-ion spin anisotropy.

Figire 2 shows the examples of behavior of weak ferromagnetic vector **F** depending on relative temperature $T/T_{N,max}$, where $T_{N,max} = 320$ K is the temperature of magnetic moment formation in the model system $YFeO_3$. What is important, the MC1 method, same as MFA, shows the presence of the magnetic moment compensation (effect of negative magnetization) at low concentration of chromium $x \approx 0.2$ (Figire 2, a), and also predicts the presence of the second compensation near concentration $x \approx 0.8$ (Figire 2, b).

In the case of the MC2 method, at certain concentrations the temperature dependences of absolute values of vectors

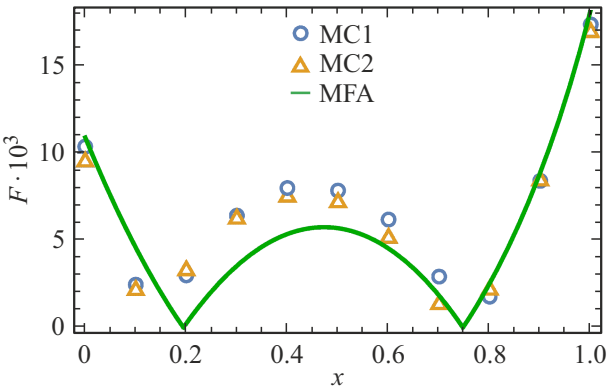

Figure 3. Concentration dependence of the value of weak ferromagnetic vector **F** in MC1 methods (circles), MC2 methods (triangles) and in the mean field approximation (solid line) near the ground state ($T/T_{N,max} \ll 1$).

F, **G** behave in the same manner as in case of MC1 method, but with the ordering temperature of $T_{N,max} = 85$ K. Besides, the magnetizations near the ground state turn out to be close, too (Figire 3). The first and second compensations, for example, at $x = 0.2$ and $x = 0.77$, accordingly, are observed here as well (Figire 4).

The specific feature of the method is the fact that in the area of intermediate concentrations at the selected parameters of the model we find phase G_{xyz}, which includes all components of vectors **F**, **G**, **A**, **C** (Figire 4). Therefore, there is angular configuration, which in the mixed composition $YFe_{1-x}Cr_xO_3$ turns out to be more preferable than the „parent one“ $\Gamma_4(G_x, A_y, F_z)$.

The MC2 method remains classical as such, but accounting for the operator nature of the spin using quasi-classical wave functions of type (8) turns out to be sufficient to show the presence of phases different from Γ_4 (i. e. the possibility of spin reorientation) only at the expense of the competition of Dzyaloshinskii vectors without inclusion of additional mechanisms, for example, external fields and

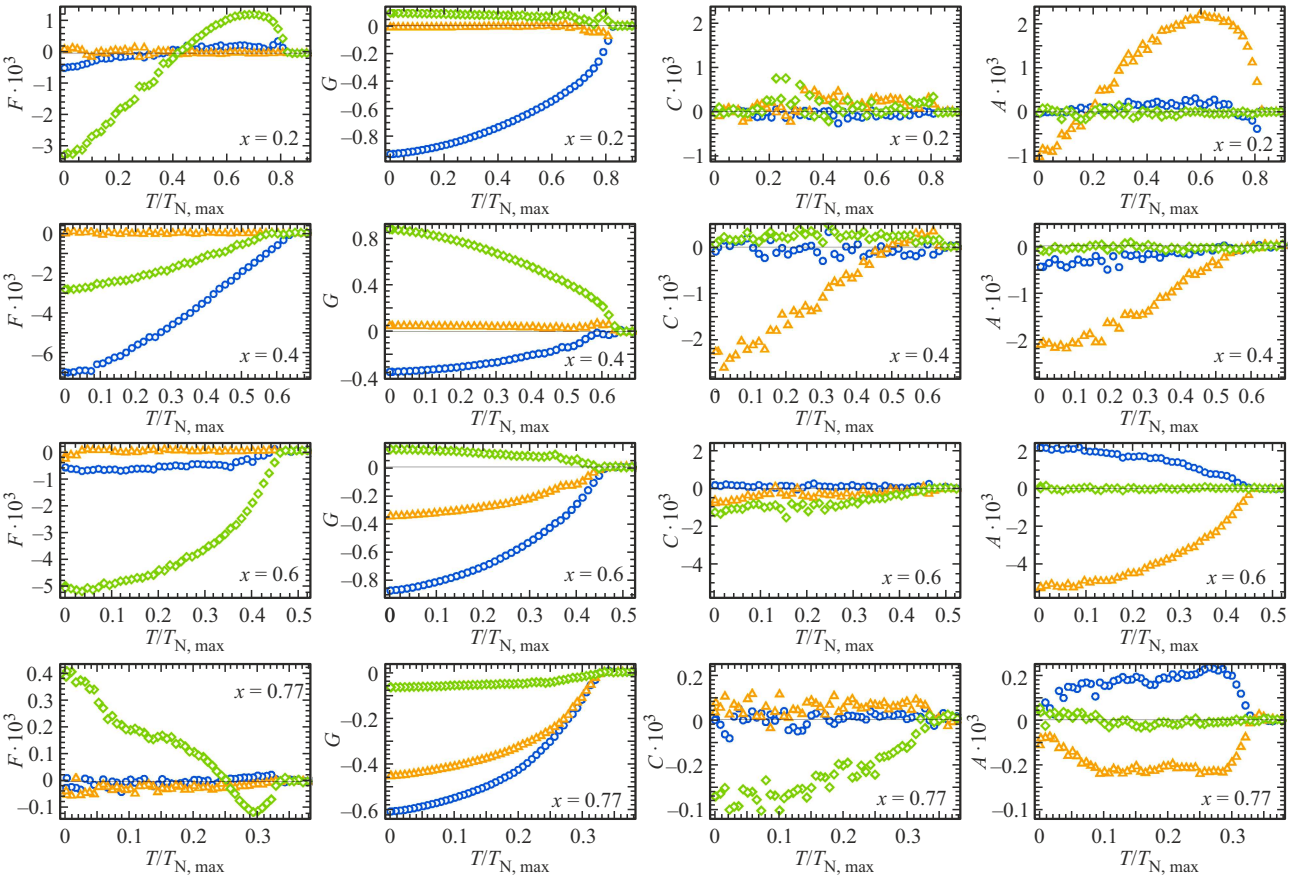

Figure 4. Temperature dependences of basis vectors at different concentrations of chromium, blue circles are the projection of the corresponding vector along a-axis of the crystal, orange triangles are onto along b-axis, green diamond are onto along c-axis.

single-ion anisotropy. The inspection of the MC2 method in the absence of competition, with the co-directional vectors $\mathbf{d}_{\mathrm{FeFe}}$, $\mathbf{d}_{\mathrm{CrCr}}$ and $\mathbf{d}_{\mathrm{FeCr}}$, found no angular configurations, only phase $\Gamma_4(G_x, A_y, F_z)$ is observed.

Note the issue of determining the critical temperatures T_C, for example, when the system transitions from the disordered paramagnetic state to phase Γ_4.

In case of classical MC methods with Metropolis algorithm these temperatures become much lower than in the case of the mean field approximation. On the one hand, it is known that MFA tends to overestimate T_C, since such methods do not account for important local correlations and fluctuations. On the other hand, when simulating systems that contain off-diagonal operators in the Hamiltonian, a strong underestimation T_C occurs in classical MC methods. We relate this to the unkillable dispersion of energy and order parameters, caused by the continuity of the spectrum of single-site operators. When a new state is selected in the site, we are limited only by the normalization condition; therefore, at any temperature a new site state will be found, which is rather close by energy, which will be most probably accepted on process of the elemental step of the Metropolis algorithm. For this reason in this paper we were interested only in the magnetic configuration of the mixed composition $YFe_{1-x}Cr_xO_3$, and the results above were given in relative temperatures $T/T_{\mathrm{N,max}}$, where $T_{\mathrm{N,max}}$ is the temperature of transition from the disordered paramagnetic state for $YFeO_3$ ($T_{\mathrm{N,max}} = 320\,\mathrm{K}$ in the MC1 method, and $T_{\mathrm{N,max}} = 85\,\mathrm{K}$ in the MC2 method). For more precise study of the critical temperatures by the classical MC method, other algorithms are required [31,33,34,38].

5. Conclusion

In this paper we developed software for simulating of magnetic moments by the Monte Carlo method in the mixed orthoferrite–orthochromite $YFe_{1-x}Cr_xO_3$. Key features are explained by the competition of the Dzyaloshinskii vectors. It is confirmed that the system has the first compensation near $x \approx 0.2$, and also the second compensation is predicted near $x \approx 0.8$. Whereas in the parent systems $YFeO_3$ and $YCrO_3$ the phase $\Gamma_4(G_x, A_y, F_z)$ is observed exclusively, and their mixed composition demonstrates an angular phase G_{xyz}, including all components of the basis vectors $\mathbf{F}, \mathbf{G}, \mathbf{C}, \mathbf{A}$. The presence of phase G_{xyz} indicates the possibility of spin reorientation, but detailed description requires additional research, accounting for single-ion spin

anisotropy, and the modification of the algorithm that determines the elemental step of the Monte Carlo method.

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Conflict of interest

The authors declare that they have no conflict of interest

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