Spin-reorientation phase transition and nonequilibrium thermodynamics of compensated ferrimagnet $ErFeO_3$

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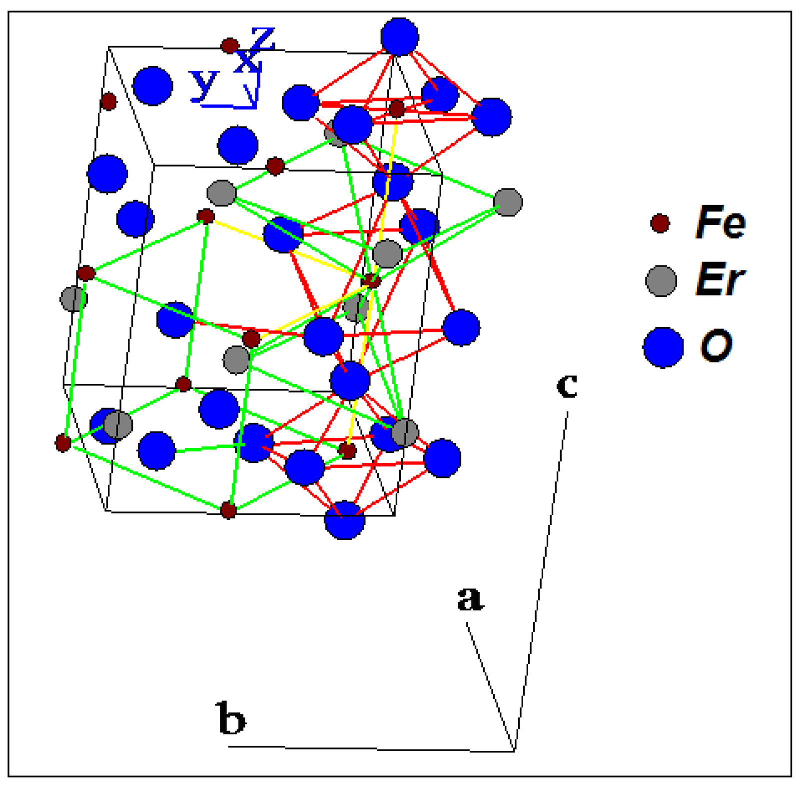
1. Introduction

Orthoferrites with a general formula RMO_3, where R and M are rare-earth and transition metal ions, have good perspectives for applications in ultrafast spin switching devices, sensors, high-frequency generators due to their unique characteristics associated with the presence of magnetoelectric coupling, negative magnetization, spin flips, and exchange bias. The compensated ferrimagnet orthoferrite $ErFeO_3$ exhibits the exchange bias (EB) effect, which was previously detected as the traditional shift of the magnetization hysteresis loops M vs H near the compensation temperature T_{comp} = 45 K[1-3].

2. Crystal structure

Erbium orthoferrite has D_{2h}^{16} space group , tetragonal system.



3. Hamiltonian of the model:

$$\hat{H}=\sum_{i_1j_2} j_{12}\boldsymbol{S}_{i_1}\boldsymbol{S}_{j_2}+\sum_{i_1j_2} b_{12}S^z_{i_1}S^z_{j_2}+\sum_{i_1j_2}\boldsymbol{D}_{12}\left[\boldsymbol{S}_{i_1}\times\boldsymbol{S}_{j_2}\right]+\sum_{ik\alpha}\tilde{j}_\alpha S_i^\alpha\sigma_k^\alpha-\mu_B g_{Fe}\boldsymbol{H}\left(\sum_{i_1}\boldsymbol{S}_{i_1}+\sum_{j_2}\boldsymbol{S}_{j_2}\right)-\mu_B\left(\sum_{k\alpha}g_\alpha H_\alpha\sigma_k^\alpha\right)$$

Here, $j_{12}>0$ – isotropic part of the AFM Fe-Fe exchange interaction, b_{12} – anisotopic part of the AFM Fe-Fe exchange, $\tilde{j}_\alpha$ - anisotropic Fe-Er exchange, $\boldsymbol{D}_{12}$ is $y||b$-component of the vector parameter of Dzyaloshinsky-Moriya interaction, $\boldsymbol{H}$ – magnetic field, g_α – anisotropic erbium g-factor , respectively.

Mean-field approximation:

$$\hat{H}_0=\hat{H}_{0Fe}+\hat{H}_{0Er}$$

$$\hat{H}_{0Fe}=\sum_i^N\left(\tilde{\boldsymbol{H}}_2\boldsymbol{S}_i\right)+\sum_j^N\left(\tilde{\boldsymbol{H}}_1\boldsymbol{S}_j\right)+H_{const},\quad \hat{H}_{0Er}=\sum_k^{2N}\tilde{\boldsymbol{H}}\boldsymbol{\sigma}_k$$

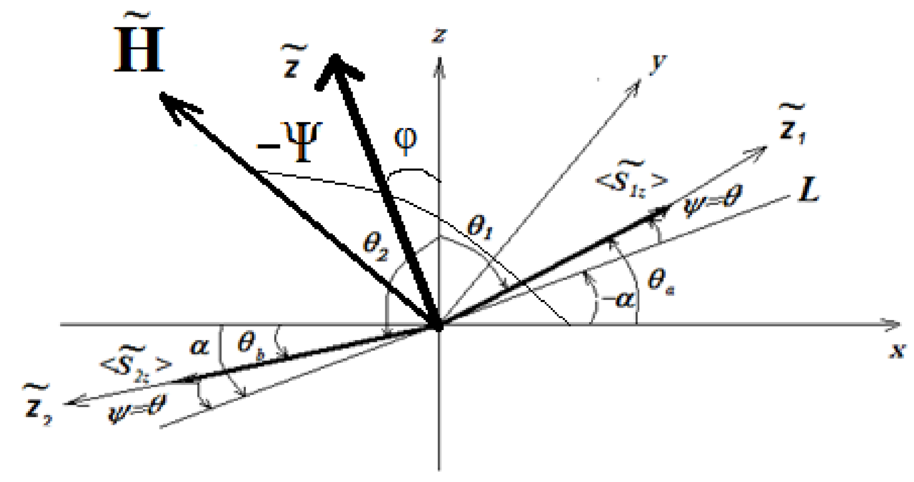
4. Results

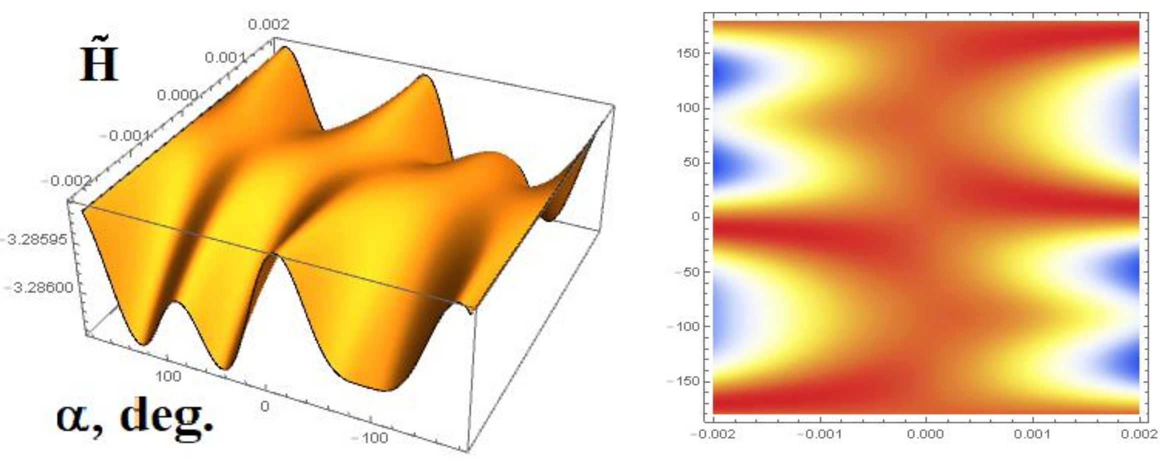
Free energy:

$$\tilde{F}(\alpha)=-\frac{1}{2}S^2\left\{\cos(2\theta)+d\sin(2\theta)-\frac{b}{2}\left(\cos(2\alpha)-\cos(2\theta)\right)\right\}-\tilde{T}\ln\left[2\cosh\left(\frac{\tilde{\tilde{h}}(\alpha)}{2\tilde{T}}\right)\right]+g_{Fe}S\sin(\theta)\tilde{H}\sin(\alpha-\psi)$$

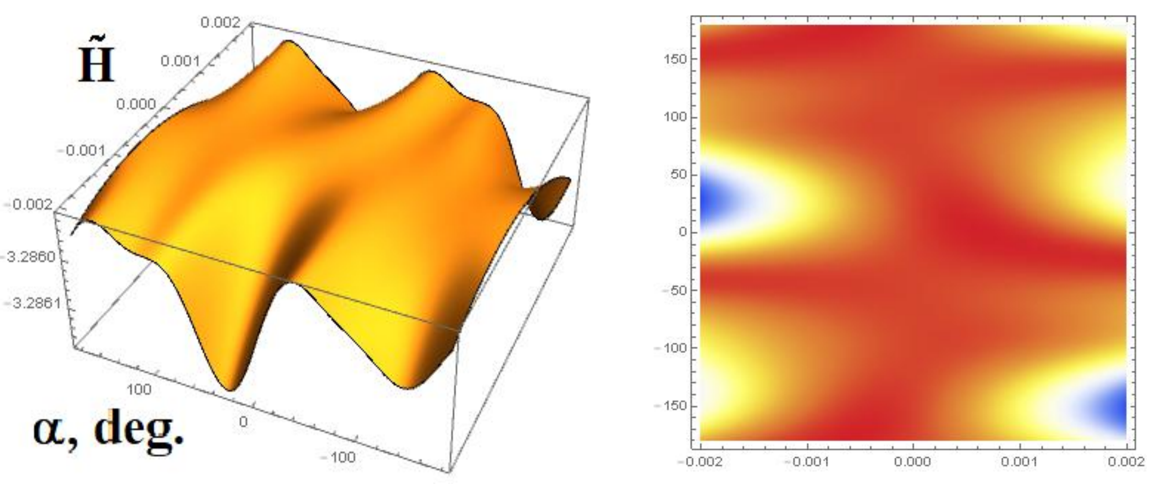
$$\tilde{\tilde{h}}(\alpha)=\sqrt{\sin^2(\alpha)\left(\frac{S}{\gamma_x}\sin(\theta)+g_a\tilde{H}\sin(\alpha-\psi)\right)^2+\cos^2(\alpha)\left(\frac{S}{\gamma_z}\sin(\theta)+g_c\tilde{H}\sin(\alpha-\psi)\right)^2}-effective\ field$$

Geometry of the quantum system in applied fields: ψ =180° H||-a

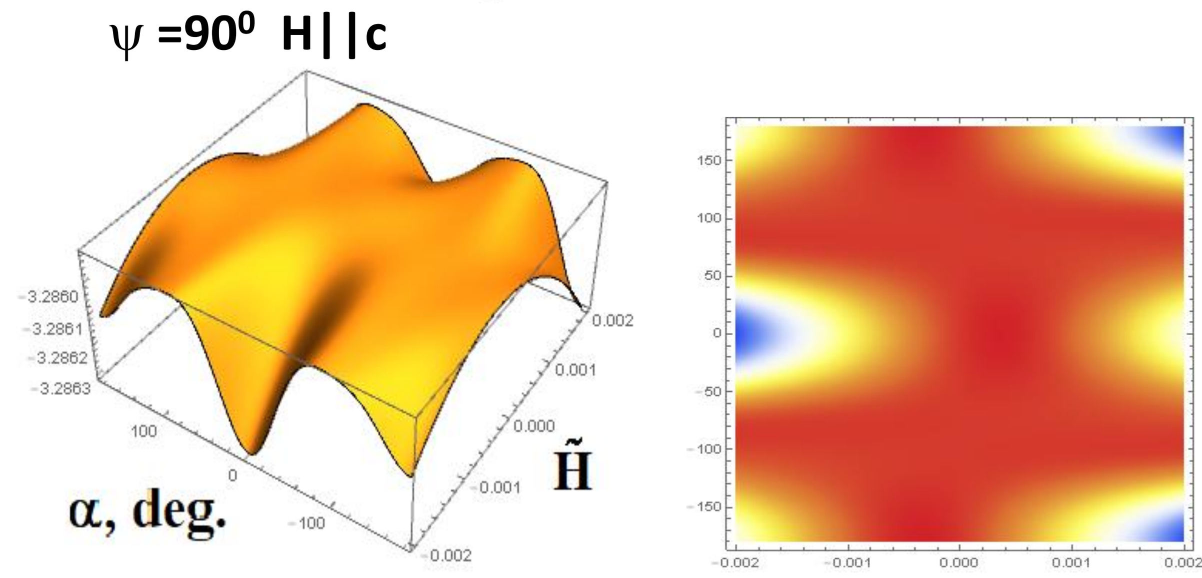




ψ =145°



ψ =90° H||c



Energy of anisotropy:

$$B(\tilde{T},\alpha)=-\frac{1}{2}bS^2\sin^2(\alpha)\left(1-\frac{\tilde{T}_{SR}}{\tilde{T}}\right)-\frac{1}{32\tilde{T}\gamma_z^2}S^2d^2$$

Temperature of the spin-reorientation phase transition:

$$\tilde{T}_{SR}=-\frac{d^2}{16b}\left[\frac{1}{\gamma_x^2}-\frac{1}{\gamma_z^2}\right]-\quad SR\ temperature$$

Compensation temperature:

$$\tilde{T}_{C,xz}(\alpha)=\frac{1}{4g_{Fe}}\left(\frac{g_a\sin^2(\alpha)}{\gamma_x}+\frac{g_c\cos^2(\alpha)}{\gamma_z}\right)$$

Canting angle:

$$\theta_0=\frac{d}{2}\cdot\frac{1}{1-\frac{1}{16\tilde{T}}\left[\frac{\sin^2(\alpha)}{\gamma_x}+\frac{\cos^2(\alpha)}{\gamma_z}\right]^2}$$

5. Conclusions

1. The model of uniformly magnetized regions (domains or superparamagnetic particles) with arbitrary $\alpha\in(-\pi,\pi)$ was considered.
2. It was suggested that the relaxation time for the whole system of magnetic particles points out on two types of spin dynamics. Coherent and incoherent spin rotations correspond to relaxation time and instant paraprocess phenomena, respectively.
3. It was shown that an applied magnetic field in the vicinity near the compensation point causes a slight instant additional canting of the transition metal magnetic moments, disrupting the balance of energies of isotropic and anisotropic exchange interactions in transition-metal and rare-earth ions subsystems. Unidirectional anisotropy, associated with the direction of the uncompensated ferromagnetic moment of transition-metal ions, arises in complete analogy with behavior of layered FM-AFM structures.

References

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[2] I. Fita, R. Puzniak, E.E. Zubov, P. Iwanowski, and A. Wisniewski, Phys. Rev. B **105** (2022) 094424.
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