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Effect of roughness on the magnetic structure of ferro/antiferromagnetic interface

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Abstract

Spin structures at the ferro/antiferromagnetic interfaces perturbed by defects such as atomic high steps are analytically investigated. A two-dimensional model is proposed to describe the spin distribution formed on the interfacial step at the domain wall. A criterion of the domain wall configuration relative to the interface is found, defined by the magnetic and geometrical characteristics of the interface and the magnet. © 2001 Published by Elsevier Science B.V.

Keywords: Anisotropy-single ion; Domain wall-structure; Interface roughness; Layered Heisenberg systems

Layered magnetic structures and interfaces between different magnetically ordered media have aroused considerable interest in recent years due to their wide variety of surprising features and a multiplicity of technological uses. The roughness of atomic high steps necessarily abundant on the interface involves severe consequences for the magnetic order of the layered systems. The intention of the present paper is to describe spin structures at ferro/antiferromagnetic (FM/AFM) interfaces perturbed by defects such as steps. We develop a model that allows one to obtain analytical expressions for the magnetic ordering throughout the volume of the system and for the energy of the domain walls (DWs) of various configurations. Information on the real spin distribution at the perturbed interface expressed in terms of the material parameters of the magnet can be used as a basis for analysis of the observable physical effects, the formation of DWs may lead to, such as exchange bias and other related phenomena.

Consider classical Heisenberg FM/AFM system with atomic high step on the interface, taking into account a weak easy-axis anisotropy γ along the x direction in the easy xz-plane (Fig. 1). As it will be seen from below, qualitative analysis of the magnetic structure, we are interested in, is allowed under the assumption of equal anisotropy for FM and AFM, however, the quantitative analysis would require one to differ anisotropy for the two layers. At the exchange interaction through the interface J_S under a critical value J^* spin ordering in FM and AFM is ideal, and collinear DW forms along one of the x half-axes. At $J^* < J_S < J^{**}$ the DW takes noncollinear form. As J_S reaches the critical value J^{**}, the DW is

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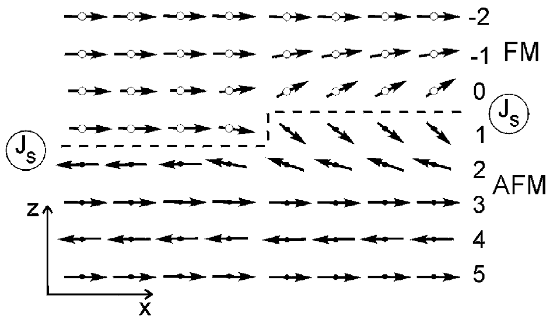

Fig. 1. DW caused by a step on FM/AFM interface given single-ion anisotropy in the easy plane (*xz*).

repelled from the interface since the energy of the DW in the layer is less than that at the interface. To find a criterion of the DW orientation and to determine the values J^* and J^{**}, calculate the energy of the noncollinear DW at the step along the interface.

From the energy of the magnetic interaction in the spin chain along the *z*-axis at fixed *x* static equations for spin deviations φ in the chain can be derived. After variables substitution taking into account "layered" ordering in AFM, linearized equations take the form:

$$J_A b^2 \frac{\partial^2 \varphi}{\partial z^2} + \frac{\gamma}{2}\sin(2\varphi) = 0,$$

$$J_F b^2 \frac{\partial^2 \varphi}{\partial z^2} + \frac{\gamma}{2}\sin(2\varphi) = 0, \quad (1)$$

where b is lattice parameter along z direction, J_A and J_F are the exchange constants in the *z*-directions in AFM and FM. Eqs. (1) is complemented by the boundary conditions

$$bJ_A \left.\frac{\partial \varphi}{\partial z}\right|_{z=-b/2} = J_S \sin(\varphi_0 - \varphi_1),$$

$$bJ_F \left.\frac{\partial \varphi}{\partial z}\right|_{z=+b/2} = J_S \sin(\varphi_0 - \varphi_1). \quad (2)$$

The solutions of Eqs. (1) describe the rotation of spins in a chain along z at fixed x:

$$\varphi = 2\arctan\exp((z_A - z)/l_A), (z<0),$$

$$\varphi = 2\arctan\exp((z_F - z)/l_F), (z>0), \quad (3)$$

where $l_A = b\sqrt{J_A/\gamma}$ and $l_F = b\sqrt{J_F/\gamma}$ are the "magnetic lengths" in the half spaces. The values z_A and z_F can be defined from the boundary conditions (2) and are the functions of the parameters J_A, J_F, J_S, γ. Using Eqs. (3) we obtain the energy of the unit length of the DW along the interface:

$$E_\parallel \approx \sqrt{J_F\gamma} + \sqrt{J_A\gamma} - \frac{\gamma}{2} + \frac{\gamma}{b}(z_F - z_A)$$

$$+ 2J_S\left(\frac{b/2 - z_F}{2l_F} + \frac{b/2 + z_A}{2l_A}\right)^2. \quad (4)$$

Energy (4) appears to be the function of the exchange integrals of FM, AFM and through the interface, depending also on the easy-axis anisotropy parameter. Common expression for the DW energy immediately follows from Eqs. (4) in the case $J_A = J_F = J_S$: $E_0 = 2\sqrt{J\gamma}$, which agrees with that obtained by the direct calculation of the DW energy in the homogeneous magnet. To compare the energies of variously configurated DW, consider the case of equal values of the exchange parameters in FM and AFM: $J \equiv J_A = J_F \neq J_S$ (we use the assumption of equal exchange constants in FM and AFM to obtain some qualitative results. Note, that, for Fe/Cr, as an example, $J_{Fe}/J_{Cr} \approx 2$ while $J_{Fe}/J_{Fe-Cr} \approx 10$ and thus the assumption is valid to be a good approximation). Then, the energy of the unit length of the DW along the interface is

$$E^0_\parallel(J, J_S, \gamma) = 2\sqrt{J\gamma} + \frac{\gamma}{2}\left(1 - \frac{J}{J_S}\right). \quad (5)$$

Comparing this expression with the energy of the collinear DW in the plane of the interface $E_{col} = 2J_S$, a critical value of the exchange interaction through the interface $J_S{}^*$ can be found, at which the transformation of the collinear DW into the noncollinear DW occurs: $J_S^* = \frac{1}{2}\sqrt{J\gamma}$. At $J_S > J^{**} = J$ the energy of the DW along the interface exceeds the energy of the DW within the thickness of the magnet, the DW is repelled from the interface and is oriented perpendicular to the interface. It is easy to obtain the value of the J^{**} for $J_F \neq J_A$: $J^{**} = \sqrt{J_F J_A}$. If the exchange parameters in FM and AFM differ, the DW at

$J_S > J^{**}$ forms, obviously, in the magnet with the smallest value of the exchange interaction. These conclusions as to DW orientation are in agreement with the results of numerical calculations for Fe/Cr multilayers presented in Ref. [1]. If the finite thickness of the FM and AFM layers and the finite distance L between the steps on the interface are take into account, a prerequisite to the formation of the DW along the interface is $E_{\parallel} L < E_{\perp} h$, where $E_{\perp} = 2\sqrt{\tilde{J}\gamma}$ ($\tilde{J}$ is the exchange integral along the x-direction). The opposite inequality is the condition of the DW formation perpendicular to the interface.

Analytical description of the nonuniform magnetization distribution caused by a monatomic step at the FM/AFM interface can be provided in the framework of a simple 2D model proposed in Ref. [2] for a system of AFM with the lattice dislocation. Consider J_S value on the interval $J^* < J_S < J^{**}$ which corresponds to noncollinear DW formation along the interface. For an equivalent system of two FM half spaces in contact after corresponding variables change, long-wave equations for the magnetization distribution take the form

$$\tilde{J}_A a^2 \frac{\partial^2 \varphi}{\partial x^2} + J_A b^2 \frac{\partial^2 \varphi}{\partial z^2} - \frac{\gamma}{2}\sin(2\varphi) = 0,$$

$$\tilde{J}_F a^2 \frac{\partial^2 \varphi}{\partial x^2} + J_F b^2 \frac{\partial^2 \varphi}{\partial z^2} - \frac{\gamma}{2}\sin(2\varphi) = 0, \quad (6)$$

where a is lattice parameter along the x direction, $\tilde{J}_F$ and $\tilde{J}_A$ are, respectively, the exchange integrals in FM and AFM in x-direction. Nonlinear Eqs. (6) can be linearized by replacing single-ion anisotropy $E_{an} = \gamma(1-\cos^2\varphi)/2$ with the piecewise parabolic function, which is possible when the exchange interaction in FM and AFM are of the same order of value. Since we are interested in the magnetization distribution over distances larger than atomic dimensions, replace an interface with a step by the ideal boundary, having reversed the sign of the exchange interaction through it on one side of the step. Complementing the boundary condition presenting the density of the effective forces acting at the interface

$$f_{\pm}(x) = \pm\,\mathrm{sgn}(x) J_S \sin(\varphi|_{z=+b/2} - \varphi|_{z=-b/2}), \quad (7)$$

leads us to the following solution of the volume problem (6):

$$\varphi(x, z>0) = -\frac{J_S}{\pi a\sqrt{\tilde{J}_F J_F}} \times \int_{-\infty}^{+\infty} \mathrm{d}x' K_0\left(\sqrt{\frac{(x-x')^2}{\sigma_x^2} + \frac{z^2}{\sigma_z^2}}\right) \sin(\chi(x'))\,\mathrm{sgn}(x') \quad (8)$$

(and the analogous expression for AFM half space), where Macdonald's function $K_0(k)$ is the Green's function of the Klein–Gordon equation; $\chi = \varphi|_{z=+b/2} - \varphi|_{z=-b/2}$ the function of relative spin deviation at the interface; $\sigma_x = a\sqrt{\tilde{J}_F/\gamma}$ and $\sigma_Z = b\sqrt{J_F/\gamma}$ are, respectively, the "magnetic lengths" along the x and z directions. From the expression (8) a 1D equation for the function $\chi(x)$ follows. In the case of the equal exchange constants in FM and AFM it takes the form

$$\chi(x) = -\pi - \frac{2J_S}{\pi a\sqrt{J\tilde{J}}} \times \int_{-\infty}^{+\infty} \mathrm{d}x' K_0\left(\sqrt{\frac{(x-x')^2}{\sigma_x^2} + \frac{b^2}{4\sigma_z^2}}\right) \sin(\chi(x'))\,\mathrm{sgn}(x'). \quad (9)$$

Eq. (9) can be solved by the successive approximations method. For the first approximation it gives:

$$\chi_1(x) = -\pi - \frac{J_S}{J^*}\sin(\varepsilon)\frac{1}{\pi}\int_{-x/\sigma_x}^{\infty} \mathrm{d}p K_0(p), \quad (10)$$

where ε changes from $-\pi$ (at $J_S = J^*$) to $-(\pi/2) \times \sqrt{\gamma/J}$ (at $J_S = J$). The function

$$I(x) = \frac{1}{\pi}\int_{-x/\sigma_x}^{\infty} \mathrm{d}p K_0(p)$$

can be estimated on the different intervals of the coordinate x values:

$$I \approx \begin{cases} \sqrt{\sigma_x/|x|}\exp(x/\sigma_x)/\sqrt{\pi}, & x \ll -\sigma_x; \\ ((1-|x|/\sigma_x) - (|x|/\sigma_x)\ln(|x|/\sigma_x))/\pi, & -\sigma_x < x < 0; \\ ((1+|x|/\sigma_x) - (|x|/\sigma_x)\ln(|x|/\sigma_x))/\pi, & 0 < x < \sigma_x; \\ 1 - \sqrt{\sigma_x/x}\exp(-x/\sigma_x)/\sqrt{\pi}, & x \gg -\sigma_x. \end{cases} \quad (11)$$

The solution of the 2D problem can be restored by substituting the solution of the 1D Eq. (9) into expression (8):

$$\varphi(x, z>0) \approx \frac{1}{2}\frac{J_S}{J^*}\sin(\varepsilon(J_S)) \times \frac{1}{\pi}\int_0^\infty \mathrm{d}p K_0\left(\sqrt{(p - x/\sigma_x)^2 + (z/\sigma_z)^2}\right). \quad (12)$$

At $x = 0$ and $z \gg \acute{o}_Z$ it follows from Eqs. (12) that $\varphi \propto (J_S/J^*)\sin(\varepsilon(J_S))\sqrt{z/\sigma_Z}\exp(-z/\sigma_Z)$. At large distances from the interface the system turns to the ground state (Fig. 1).

In conclusion, a two-dimensional model is presented for analytical description of the spin structure at the FM/AFM interface with the atomic high step. The domain wall is necessarily associated with the step on the interface. The energy along with the orientation of the domain wall is dictated by the anisotropy and exchange parameters of the FM, AFM and through the interface as well as by the thickness of the layers and geometry of the interface. The distribution of magnetization in the entire volume of the magnet containing the domain wall along the interface is expressed in the terms of the magnetic and geometrical parameters of the system. Decrease of the nonuniformity of the magnetization distribution into the depth of the magnets is exponential, and the width of the domain wall is proportional to the exchange interaction in the magnets and inversely related to the anisotropy parameter.

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