Phase Diagram of Multilayer Magnetic Structures

V.D. Levchenko
M.V. Keldysh Institute for Applied Mathematics, Russian Academy of Sciences

A.I. Morosov and A.S. Sigov
Moscow State Institute of Radioengineering, Electronics, and Automation (Technical University)

I. INTRODUCTION

Multilayer magnetic structures have attracted widespread attention after discovery of the phenomenon of giant magnetoresistance. Within the span of eleven years a great many of papers devoted to the multilayer structures has been published. Considerable recent attention has been focused on multilayer “ferromagnet–layered antiferromagnet” structures. An example of such structures, according to recent experiments on neutron diffraction, is given by multilayer Fe/Cr structures, in which antiferromagnetic chromium layers of the thickness $d < 4.5 \text{nm}$ consist of ferromagnetic atomic planes with antiparallel orientation of spins in adjacent planes. The spins of chromium atoms lie in these planes, the plains in their turn being parallel, on the average, to the layer interfaces. An analogous structure has been observed in manganese layers in multilayer Fe/Mn structures.

In multilayer “ferromagnet–layered antiferromagnet” structures, the exchange interaction between ferromagnetic layers is caused mainly by the interaction via antiferromagnetic order parameter, whereas the RKKY interaction far away from the Neel temperature provides only a small additive to the first one. To describe the interaction via antiferromagnetic order parameter, Slonczewski proposed a phenomenological model of “magnetic proximity” in whose context the layers of ferromagnet are assumed to be magnetized practically uniformly and considerable distortions of the order parameter are supposed to take place only in the layers of antiferromagnet.

The presence of atomic steps at layer interfaces that change the local thickness of the antiferromagnet by one monoatomic layer gives rise to frustrations in the system (Fig. 1a). In this case the uniform distribution of the order parameters in the layers does no longer correspond to the energy minimum.

If the characteristic distance between atomic steps at the layer interface (we shall call it the step width $R$) exceeds some critical value, it becomes energetically favorable to break the layers up into domains (Fig. 1b). The domain boundaries in layer planes coincide with the atomic step edges. It should be noted that the magnitude of $R$ strongly depends on the technology conditions.

Recent investigations on the state of ferromagnetic iron film on the rough (001) chromium surface have shown the presence of several magnetic phases depending upon the film thickness and roughness rate (the value of $R$).

All the aforesaid bears witness to considering the problem of “thickness-roughness” phase diagram of “ferromagnet–layered antiferromagnet” magnetic structures as a high priority task.

The paper has the following structure. The consideration begins with a simple model that allows one to describe the behavior of the system in question qualitatively. In the third section one can find model results on the phase diagram of the two-layer system: thin ferromagnetic film on antiferromagnetic substrate (or vice versa). The phase diagram for “ferromagnet–antiferromagnet–ferromagnet” three-layer structure is found and discussed in the fourth section, the treatment being possible to be generalized to multilayer. In conclusion the main results are adduced.

II. DESCRIPTION OF THE MODEL

When describing the multilayer structure, we restrict ourselves to the mean-field approximation. Let us introduce the order parameter for each magnetic layer: the magnetization vector for the layers of ferromagnet and antiferromagnetism vector, equal to the difference in magnetization vectors of the sublattices, for the layers of antiferromagnet.

It is known that in sufficiently thin magnetic layers with the thickness of some nanometers, the atomic spins lie in the layer planes. Therefore, at $T < T_C$, $T_N$ (here $T_C$ is the Curie temperature for single ferromagnetic lay-
ers, and $T_N$ is the Neel temperature of antiferromagnetic layers), it is possible to describe the local value of the order parameter in the layer planes by the angle $\theta$ of the order parameter vector with a certain given axis in the layer plane. The order parameter modulus is assumed to remain unchanged in each layer.

In the framework of the assumptions made above, the exchange energy $W_i$ caused by a nonuniformity within the $i-$th layer can be introduced as

$$ W_i = \frac{J_i S_i^2}{2b_i} \int (\nabla \theta_i)^2 \, dV, \quad (1) $$

where the integral is taken over the $i-$th layer volume, $J_i$ is the exchange stiffness, $S_i$ is the mean spin of the atom, $b_i$ is the inter-atomic distance.

By varying Eq. (1) with respect to $\theta_i$ we get the equation for the order parameter distribution in the layer:

$$ \Delta \theta_i = 0. \quad (2) $$

To obtain the true boundary conditions one needs a more exhaustive procedure. Owing to frustrations arising at the layers boundaries the difference $\theta_i - \theta_{i+1}$ can become large enough at the interlayer boundary, whereas inside the layers the frustrations are absent, the value of $\theta_i$ varies smoothly, and the difference of $\theta_i$ values in the nearest cells is small. That is why, when calculating exchange energy within the X-Y model, we may expand cosine of the difference of the angles $\theta_i$ in neighboring cells in power series if the cells belong to the same layer, but we’ll not do that if the cells belong to different layers. By differentiating the energy with respect to the quantity $\theta_i$ in the cell lying in the layer boundary, we come to the equation which takes the following form as one passes to the continuous representation:

$$ \Delta \theta_i - \frac{\partial \theta_i}{\partial n} = \pm \frac{J_{f,af} S_{i+1}}{J_i S_i} \sin (\theta_i - \theta_{i+1}), \quad (3) $$

where $\Delta$ is the two-dimensional Laplacian in the layer plane, $\frac{\partial}{\partial n}$ is the derivative in the direction of the outer normal to the interface plane, the exchange constant $J_{f,af}$ describes the interaction of spins corresponding to different layers, and all distances are normalized to the value of $b_i = b$ which is assumed to be the same in all layers. The signs in the right-hand part of Eq. (3) are opposite for different sides of the atomic step at the interface. For the free surface of the layer the right-hand side of Eq. (3) equals zero.

The energy of exchange interaction between adjacent layers takes the form

$$ W_{i,i+1} = \pm \frac{J_{f,af} S_i S_{i+1}}{b^2} \int \cos (\theta_i - \theta_{i+1}) \, dS, \quad (4) $$

where the numbers $i$ and $i + 1$ denote corresponding layers, the integration is performed over the interface of the layers, and the sign in the right member coincides with that one in Eq. (3).

By varying the energy of interlayer interaction represented in terms of the continuum model distribution one gets an equation similar to Eq. (3) but without the first summand in the left-hand side. This renders it impossible to pass from Eq. (3) to Eq. (2) if adjacent layers are identical in composition.

The atomic steps divide the whole interlayer surface into regions of two types: in the regions of the first type the surface energy takes its minimum for $\theta_i = \theta_{i+1}$ and in the regions of the second type the energy is a minimum for $\theta_i = \pi - \theta_{i+1}$.

To find the order parameters distributions in the multilayer structure it is necessary to solve the system of differential equations (3) with boundary conditions (2).

Now let us take up the applicability of this simple model to real multilayer structures. The continuum approximation is valid only in the case that characteristic measures of the problem are much higher than the interatomic distance. The layer thicknesses in multilayer structures as well as the distances between atomic steps are of about several nanometers, so they may be considered as far exceeding the lattice parameter. Hence the continuum approximation is applicable for estimations and qualitative treatment.

In the model proposed, the exchange interaction is assumed to be isotropic, i.e. identical in the plane and in perpendicular direction. The model with anisotropic exchange interaction is reduced to the given one by renormalization of the distance scale in any of two non-equivalent directions.

An interdiffusion of atoms from neighboring layers leads only to renormalization of $J_{f,af}$, if the region of mutual stirring extends up to several monolayer structures, i.e. is of atomic size scale. This constant value is obtained by microscopic calculations.

Eqs. (3), (4) are written in the exchange approximation, but can be easily generalized to the case of small anisotropy in the layer plane.

**III. THE METHOD OF CALCULATIONS**

Let the atomic step edges be rectilinear and parallel to each other. The $x$-axis of the coordinate system lies in the layer plane and is perpendicular to the step edges, and the $z$-axis is perpendicular to the layer plane (two-dimensional case).

The assumed set of equations includes Laplace equations (3) for the each plane layer $-\infty < x < \infty, \, 0 < z < a_i$, where $i = 1 \ldots n$ is the layer number and $a_i$ is the layer width, the boundary conditions (3) at interlayer surfaces being nonlinear and discontinuous. For numerical calculations we reduce this set to the system of unidimensional integral equations.

We require the function $\theta_i(x, z)$ to be continuous inside the region $0 < x < L, \, 0 < z < a_i$ (here $L$ is half of the modeling region length along $x$ axis), and additionally
The equation for zeroth–order Fourier coefficients has the form of Eq. (3) as the Fourier series:

\[ L \] and step \( \Delta x \) with boundary conditions

\[ \sigma \]

ary conditions (8). As a result one has

where

\[ \Psi_0^+ = \frac{1}{2L} \int_{-L}^{L} \delta \theta(x) dx \]

and the variation

\[ \delta \theta(x) = \delta \theta(x) - \overline{\delta \theta}, \]

it is possible to find

\[ 0 = \int_{-L}^{L} \sigma(x) \sin(\widetilde{\delta \theta}(x) + \overline{\delta \theta}) dx \]

\[ = \cos \overline{\delta \theta} \int_{-L}^{L} \sigma(x) \sin \delta \theta(x) dx \]

\[ + \sin \overline{\delta \theta} \int_{-L}^{L} \sigma(x) \cos \delta \theta(x) dx. \]

Hence the average angle is

\[ \overline{\delta \theta} = n \pi - \arctan \left( \frac{\int_{-L}^{L} \sigma(x) \sin \delta \theta(x) dx}{\int_{-L}^{L} \sigma(x) \cos \delta \theta(x) dx} \right). \]

With Eqs (3-4) and (9-10) one can obtain the desired integral equation for the function \( \delta \theta_i \):

\[ \delta \theta_i(x) = \overline{\delta \theta}_i + \sum_{k=1}^{N} e^{i \pi k x} \frac{1}{2L} \int_{-L}^{L} e^{-i \pi k x} \xi d \xi \times \left[ K_{i+1,k}(0) \sigma_{i+1} + K_{i+1,k}(0) \sigma_i^+ \sin \delta \theta_{i+1} + K_{i,k}(a_i) \sigma_i^- \sin \delta \theta_{i-1} - K_{i,k}(a_i) \sigma_i^+ \sin \delta \theta_i \right] \equiv \hat{I}(K, \delta \theta_i, \delta \theta_i \pm 1). \]

To solve this equation numerically we use a simple iteration procedure

\[ \delta \theta_i^{n+1} = (1 - F_i(x)) \delta \theta_i^n + F_i(x) \hat{I}(F_i K, \delta \theta_i^n, \delta \theta_i \pm 1) \]

with \( 0 < F(x), F_k \leq 1 \) which are filters providing stability of the procedure and increasing its convergence rate.

The iteration procedure is over when the residual solution

\[ \varepsilon = \max \left| \delta \theta_i^n(x) - \hat{I}(\delta \theta_i^n, \delta \theta_{i \pm 1}) \right| \]

becomes less than a given value (normally, \( \varepsilon < 10^{-6} \)).

Then the solution over the whole region can be reconstructed from the formula:

\[ \theta_i(x, z) = \overline{\delta \theta}_i + \sum_{k=1}^{N} e^{i \pi k x} \frac{1}{2L} \int_{-L}^{L} e^{-i \pi k x} \xi d \xi \times \left[ K_{i+1,k}(z) \sigma_{i+1} \sin \delta \theta_{i+1} + K_{i+1,k}(z) \sigma_i^+ \sin \delta \theta_i \right] \]
As an initial approximation, one can take the function of the form
\[ \delta \theta_i(x) = \pi \sum_j \pm \eta(x - x_j), \]
where \( \eta(x - x_j) \) is a unit stepwise function with a jump at the position of crystal lattice defect location \( x_j \) and the sign \( \pm \) means that the given function can enter the sum with both plus and minus signs. As a result, one has \( N \) possible initial approximations, where \( N \) is the number of defects in the region under calculations. It should be noted that to each of the initial conditions there can correspond one of the solutions of initial nonlinear equation (a local minimum of potential energy). To find the number of defects in the region under calculations. It should be noted that to each of the initial conditions there can correspond one of the solutions of initial nonlinear equation (a local minimum of potential energy). To find the global minimum, it should be compared the energies corresponding to all of the solutions obtained.

The solution depends on the values of \( a_i \), characteristic distance \( R \) between the edges of the steps, and the parameter
\[ \alpha_f = \frac{J_{f,af} S_{af}}{J_f S_f} \]
characterizing the ratio of the exchange interaction energies of the nearest spins belonging to different layers and to ferromagnetic layer, respectively, and also the parameter \( \alpha_{af} \) defined by Eq. (11) with the subscript substitution: \( f \leftrightarrow af \).

### IV. THIN FERROMAGNET FILM ON ANTIFERROMAGNET

Let us consider a thin ferromagnet film of the thickness \( a \) (in normalized unitless scale) on the surface of layered antiferromagnet. The problem of antiferromagnet film on ferromagnetic substrate is easily reduced to the given one.

Three different states of the film-substrate system are possible, depending on the relationship between indicated parameters. If the atomic steps on the film-substrate interface are well away one from another, the frustrations give rise to domain formation. The magnetization orientation in each domain is conditioned by the surface energy minimum (Fig. 1b). Hence the magnetizations in the neighboring domains are antiparallel. The structure of Neel walls demarcating the domains depends on the value of dimensionless parameter \( \gamma \) equal to the ratio of exchange energies in the film and in the substrate:
\[ \gamma = \frac{J_f S_f^2}{J_{af} S_{af}^2} = \frac{\alpha_{af}}{\alpha_f}. \]

We have already considered the case where the order parameter distortions in the substrate are negligible. Such an approximation conforms to \( \gamma \ll 1 \). A distinguishing feature of the domain wall arising is an increase in its width with a distance from the edge of the atomic step giving rise to the wall. The parameter \( \alpha_{af} \) therewith plays an important part in the wall width behavior. The width of the domain wall \( \delta(z) \) is interpreted as the distance between the points with coordinates \( (x_1, z) \) and \( (x_2, z) \), which correspond to \( \theta_1 = \pi/4 \) and \( \theta_2 = 3\pi/4 \), respectively.

If \( \alpha_{af} \ll 1 \), the wall width \( \delta \) dependence on \( z \) is of no significance and one has a one-dimensional problem. The wall width magnitude \( \delta_f \) can be estimated from the following simple consideration.

The \( |\nabla \theta| \) value inside the wall is of the order of \( \delta_f^{-1} \).

Estimating the energy \( W_1 \) (Eq. (I)) per the domain wall unit length, one obtains
\[ w_1 \approx \frac{J_f S_f^2 a}{b \delta_f}. \]

At the same time, the spins on the interface are frustrated in the region \( |x| \lesssim \delta_f \), resulting in the energy increase in excess of the minimum by the value
\[ w_2 \approx \frac{J_{f,af} S_{af} \delta_f}{b} \]
for the domain wall unit length.

Minimizing the sum \( w = w_1 + w_2 \) one finds
\[ \delta_f \approx \sqrt{a/\alpha_f}, \]
and the domain wall energy per unit length is
\[ w \approx \frac{J_f S_f^2}{b \sqrt{a/\alpha_f}} \sim S_f \sqrt{a J_f J_{f,af} S_f S_{af}/J_{af} S_{af}}. \]

The precise numerical calculations of \( \delta_f \) and \( w \) values for a wide range of parameters \( \alpha_f \) and \( a \) confirm the estimations given above (the same relates to all cases considered below).

If \( \alpha_{af} \gg 1 \), the domain wall width essentially increases as compared to the value of \( \delta_f^0 \) at the interface. The \( \delta_f(z) \) characteristic dependence is shown in Fig. 2. The increase is practically linear \( (\partial \delta_f/\partial z \approx 1) \), with slowing down nearly to zero at a free surface of the film.

One can find the values of \( \delta_f^0 \) and \( w_1 \) using the approach analogous to that proposed for the case \( \alpha_{af} \ll 1 \). In the region \( \delta_f^0 \ll \rho \ll a \) the value of \( |\nabla \theta| \) is proportional to \( \rho^{-1} \), where \( \rho \) is the distance from the step in the \( x \) plane, just similar to the Kosterlitz-Thouless vortex. The value \( w_1 \) is equal to
\[ w_1 \approx \frac{\pi J_f S_f^2}{2 b} \ln \left( a/\delta_f^0 \right), \]
and \( w_2 \) is given by Eq. (14) with substitution of \( \delta_f^0 \) instead of \( \delta_f \). After minimization one has
\[ \delta_f^0 \approx \frac{1 + \alpha_f}{\alpha_f}, \]
\[ \delta_f(a/2) \approx a, \]
and \( w \approx w_1 \gg w_2 \).

The value of \( \delta_0^f \) is of the order of interatomic distance, and a mean wall width comprises tens of angstroms, i.e. the domain walls resulting from frustrations are much more narrow than “normal” domain walls in ferromagnets whose width is due to a competition between the exchange and anisotropy energies.

In the case of iron film on chromium substrate considered in this paper, the value of \( \gamma \) is high, \( \gamma \gg 1 \). For such conditions the domain wall structure is more complicated because the order parameter distortions can extend to the substrate as well.

If \( \alpha_f \gamma a \ll 1 \), the order parameter distortions in the substrate are small and the domain wall characteristics do not differ from those in the case \( \gamma \ll 1 \), \( \alpha_f a \ll 1 \).

For \( \alpha_f \gamma a \gg 1 \), as one can see from the results of modeling (Fig. 3), two characteristic lengths come into account: the first one \( \delta_0^f \) is the domain wall width in the substrate near the interface, and the second one \( \delta_f \) is the domain wall width in the ferromagnetic layer. Since \( \delta_f \gg a \), one can neglect the domain wall widening in the ferromagnet.

Let us consider the order parameter behavior in the antiferromagnet and the situation at the film-surface interface. Let the atomic step on the interface coincide with the \( y \)-axis of Cartesian coordinate system. For \( x < -\delta_f \) the conditions \( \theta_f = \theta_{af} = 0 \) are fulfilled, and for \( x \gg \delta_f \) the conditions \( \theta_f = 0, \theta_{af} = \pi \) are met. It follows from the symmetry of the problem that \( \theta_{af} = 0, \theta_f = \pi/2 \) for \( x = 0 \). The width of the region at the film-surface interface where the value of \( \theta_f - \theta_{af} \) differs from its optimum (0 for \( x < 0 \) and \( \pi \) for \( x > 0 \)) equals \( \delta_0^f \). In the region of \( |x| \lesssim \delta_f \) and \( |z| \lesssim \delta_f \) there arise distortions of the order parameter in the substrate (Fig. 3).

Analogously to the previous consideration one can estimate the energy \( w_1 \) inside the film by Eq. (13) and inside the substrate as

\[
w_{1f}^a \approx \pi \frac{J_{af}^2}{b} \ln \frac{\delta_f}{\delta_0^f},
\]

(20)

The energy \( w_2 \) is given by Eq. (14) with \( \delta_{0f}^a \) instead of \( \delta_f \). After minimization one has

\[
\delta_{0f}^a \approx \frac{1 + \alpha_{af}}{\alpha_{af}} \delta_f,
\]

(21)

and \( w \approx w_{1f}^a \), so the main contribution being caused by the order parameter distortions in the substrate.

The foregoing estimations relate to the case of well away distances between the steps. If the distance between the steps decreases and becomes less than the critical value \( R_c = \delta_f \), the domain walls begin to overlap and the film switches to a single domain state. The transition from a polydomain state to a single-domain state is continuous and, in the strict sense, is not a phase transition.

If \( \gamma \ll 1 \), \( \alpha_f a \gg 1 \) and \( \delta_0^f \ll R \ll \delta_f \), a static spin vortex arises in the film near the substrate enclosing the area \( z \lesssim R \).

But if \( \gamma \gg 1 \), \( \alpha_f a \gamma \gg 1 \), and the value of \( R \) is in the range \( \delta_0^f \ll R \ll \delta_f \), a similar spin vortex arises near the interface in the substrate. Near the interface spin orientation in the vortex corresponds to the minimum of the interface energy \( w_2 \). Far from the interface spin orientation is homogeneous. The results of modeling are introduced in Fig. 4.

For all others cases the distortions of order parameters are small in both the film and the substrate and their values can be considered as constants.

As it was already mentioned, the steps divide the whole interface into the areas of two types. If the mean magnetization vector makes an angle \( \psi \) with the antiferromagnetic order parameter in the substrate volume, then the value of \( \theta_f \) (or \( \theta_{af} \)) changes from zero to \( \psi \) in the vortex occupying the first type area, whereas in the vortices occupying the second type areas the value of \( \theta_f(\theta_{af}) \) changes from \( \psi \) to \( \pi \).

By an analogy to the “magnetic proximity” model the energy of the system can be written down as

\[
W = C_1 \psi^2 + C_2 (\pi - \psi)^2,
\]

(23)

where the ratio of phenomenological constants \( C_1 \) and \( C_2 \) is proportional to the ratio of the areas of both types (\( \sigma_1 \) and \( \sigma_2 \) correspondingly). If the distributions of these areas in sizes for each type are equal, one has

\[
C_1 \approx \frac{J_{f(af)}^2 S_{f(af)}^2 \sigma_f}{R b}.
\]

(24)

In the case of \( \sigma_1 = \sigma_2 \), without regard for the energy of anisotropy induced by the steps, in both the vortex phase and the region of small distortions the equilibrium magnetization of the film must be perpendicular to the antiferromagnetic order parameter. The phase diagram of the two-layer system is exhibited in Fig. 4.

This specific pattern correlates well with the results of paper 13 where the “thickness–vicinal angle \( \beta \)” phase diagram for iron film on Cr (001) surface was investigated. For \( \beta \) angles close to zero a polydomain phase was observed for the film thickness \( a < a_c = 3.5 nm \). For the film of the critical thickness \( a_c \) the characteristic distance between the edges of random steps fits the value \( \gamma a_c \). In thicker films a single-domain phase was observed, with magnetization perpendicular to the step edges. The theory proposed above predicts the antiferromagnetism vector to be parallel to the step edges, its experimental verification being of immediate interest.

If \( \beta \neq 0 \), regularly distributed parallel steps are added to random atomic steps. When the concentration of regular steps becomes dominating \( \beta \geq 1^\circ \), the critical thickness \( a_c \) falls down. It follows from our theory that \( a_c \sim R \sim t \gamma^{-1} \beta \sim \beta^{-1} \).

At high values of \( \beta \) the orientational phase transition to the phase with magnetization parallel to the steps takes
place. This transition is caused by the anisotropy induced by the steps through relativistic effects, for example, dipole interaction.

V. MULTILAYER “FERROMAGNET-ANTIFERROMAGNET” STRUCTURE

Let us consider for simplicity a three-layer system consisting of two ferromagnetic layers and an antiferromagnetic interlayer. In view of a number of various parameters, we restrict ourselves to the case of $\gamma \gg 1$ and the layers of equal thicknesses. Such a system can occur in three different states.

A-phase

At high values of $R$ all layers are divided into domains with parallel and antiparallel orientation of magnetizations in ferromagnetic layers. The domain walls penetrate into all three layers, their coordinates in the layer plane coincide with the atomic steps edges on each of two interfaces. The magnetizations of ferromagnetic layers rotate to different sides in the domain wall. The antiferromagnetic order parameter rotates together with the magnetization of that magnetic layer whose interface is free of a step in the given place.

The structure and energy of the domain wall depend on the parameter $\alpha f$. When $\alpha f a \ll 1$, one can neglect the dependence $\theta f (a f) (z)$, i.e. the domain wall widening (Fig. 3).

The consideration analogous to the case of the film gives the expression $\Delta f$ for the domain wall width in the ferromagnet and $\delta f = \sqrt{\alpha f} \approx \delta f / \sqrt{\gamma} \ll \delta f$ for antiferromagnet one. The main contribution to the domain wall energy $w_1$ comes from the ferromagnetic layers and $w$ is given by Eq. (16).

But if $\alpha f a \gg 1$, then, as in the case of a two-layer system, two length scales come into existence: $\delta f = (1 + \alpha f) / \alpha f$ and $\delta f / \sqrt{\gamma}$ which differs from that given by Eq. (21) because the distortions of the antiferromagnetic order parameter are now limited by the layer thickness. The distribution of the order parameters in this wall is shown in Fig. 6.

The domain walls in ferromagnetic layers have the width much higher than $a$, thus it may be considered as a constant across the layer. In antiferromagnetic interlayer one can see two regions (Fig. 6). In the first one $|x| \lesssim a$ the situation is analogous to the two-layer system: $|\nabla \theta| \propto a^{-1}$. The contribution of the region to $w^{(1)}_f$ is

$$w^{(1)}_f \approx \pi J f S^2_{af} \ln \frac{a}{\delta f}.$$  \hspace{1cm} (25)

But in the second region $a \ll |x| \ll \delta f$ the lines of constant $\theta$ values are almost parallel to the interfaces. In this region $|\nabla \theta| \propto a^{-1}$. The contribution of the region to $w^{(2)}_f$ is

$$w^{(2)}_f \approx \frac{J f S^2_{af}}{b a}.$$  \hspace{1cm} (26)

Taking into account the contribution to $w_1$ from ferromagnetic layers (Eq. (23)) and the interface energy $w_2$ one comes to the result given by Eq. (21) for $\delta f$, $\delta f \approx a \sqrt{\gamma}$, \hspace{1cm} (27)

and

$$w \approx \frac{J f S^2_{af}}{b} \left( \sqrt{\gamma} + a \frac{1}{\delta f} \right).$$  \hspace{1cm} (28)

B-phase

Since the magnetic rigidity of ferromagnetic layers is higher than that of antiferromagnetic ($\gamma \gg 1$), the transition to a state with practically uniform ferromagnetic layers, because of the domain walls overlapping, takes place with the distance $R$ decreasing and reaching the value $R_0 = \delta f (\delta f')$. An additional energy is associated with either distortions in antiferromagnetic interlayer or peculiarities of the structure at the interfaces. Near the Neel temperature of an interlayer $T_N$ ($T_N$ is less than the Curie temperature of ferromagnet) one has $\gamma \propto T_N / (T_N - T)$, so the transition $A \rightarrow B$ may be performed by heating the system from an initial temperature $T_0 < T_N$. The “magnetic proximity” model proposed by Slonczewski is appropriate just in that $R$ range where the $B$-phase exists.

In the range of distances $a, \delta f \ll R \ll R_0$, the energy dependence on the angle $\psi$ between the magnetizations of ferromagnetic layers is described by Eq. (23). Really, for $\alpha f a \gg 1$, in the regions of the first type (where parallel orientation of ferromagnetic layers magnetizations is energetically favorable) the antiferromagnetic order parameter changes linearly with $z$ from one interface to another by the $\psi$ value ($|\nabla \theta| = \psi / a$). In the regions of the second type (where antiparallel orientation of ferromagnetic layers magnetizations is energetically favorable) it changes by $\pi / \psi$, $|\nabla \theta| = (\pi / \psi) / a$. The frustration at interfaces is absent. The boundary energy between regions of the first and the second types is of no significance in the case $R \gg a$.

In the case $\alpha f a \ll 1$ the antiferromagnetic order parameter is almost constant, but one has frustrations at the interfaces. The jump of $\theta$ value equals $\psi / 2$ at each interface in the regions of the first type and $(\pi / \psi) / 2$ in the regions of the second type. The excess energy $w_2$ per two-dimensional unit cell in the regions of the first and the second type equals:
\[
\tilde{w} = \frac{4J_{f,af}S_fS_{af}}{b^2} \sin^2 \frac{\psi}{4},
\]
\[
\tilde{w} = \frac{4J_{f,af}S_fS_{af}}{b^2} \sin^2 \frac{\pi - \psi}{4}.
\]

Eqs. \((29,30)\) are not identical to Eq. \((23)\), the phenomenological constants \(C_1, C_2\) can be estimated by comparing energy difference of collinear and 90° orientations in the model proposed here and in the magnetic–proximity model:

\[C_{1,2} = \left( \frac{J_{f,af}S_f^2}{2\pi} \right) \frac{\sigma_{1,2}}{\sigma_{af}a} \alpha_{af} \gg 1, \]
\[\alpha_{af}a \ll 1,
\]

where \(\sigma_{1,2}\) are the areas of the first and second types on the layer surface. For \(\sigma_1 = \sigma_2\) the energy minimum is attained at \(\psi = \frac{\pi}{4}\), i.e., the magnetizations of ferromagnetic layers are mutually perpendicular in the absence of an external magnetic field.

Ferromagnetic layers are, to be sure, not ideally homogeneous. By analogy to Ref. \[\text{[32]}\], the change of the quantities \(\theta_i, \psi\) across the length of \(R\) can be shown to be of the order of \(R/\delta f(\delta_j')^2 \ll 1\).

Since the radius of the vicinity influencing the value of \(\theta_i, \psi\) at a given point equals \(\delta f(\delta_j')\), the deviation of \(\theta_i, \psi\) from their mean values is defined by the fluctuation of the quantity that characterizes the relation between the square areas of the regions of two types. If the regions of the first type dominate in given vicinity, one has \(\psi < \pi/2\), but if those of the second type, one has \(\psi > \pi/2\).

The characteristic area bounded on by the steps on the layer surface is of the order of \(R^2\), so the number \(N\) of the regions in the area \(\delta f(\delta_j')^2\) is of the order of \(\left[\frac{\delta f(\delta_j')}{R}\right]^2\). When it is assumed that the regions of both types are randomly distributed the predominance of the regions of one-type measures \(\sqrt{N} \approx \delta f(\delta_j')/R\). Therefore the characteristic fluctuation of the quantities \(\theta_i\) and \(\psi\) is of the order of \(R/\delta f(\delta_j') \ll 1\).

In the \(A\)-phase the energy of the system does not depend on the direction of the order parameter rotation in the domain wall. A different picture is observed in the \(B\)-phase: when the walls overlap one another, the degeneration in the rotation direction is eliminated and a number of metastable states arise. They differ from each other by the direction and the value of the angle of rotation of antiferromagnetic order parameter in individual areas bounded by the atomic steps.

And what is going on with further \(R\) decreasing? If \(\alpha_{af}a \ll 1\) and \(\delta f \in R \ll \delta_{af}\), the system arrives at the region of small distortions where the order parameters are practically uniform, the magnetizations of ferromagnetic layers being mutually perpendicular and the constants \(C_{1,2}\) lowering by a factor of \((R/\delta_{af})^2\) comparing to their estimations \([31]\).

\section*{C-phase}

Now let us consider the range of small \(R, R \ll a\). For such a case all distortions are localized near the interfaces, the interaction between ferromagnetic layers becomes weak and the main part is played by the energy of interaction between the neighboring layers demonstrated above with an example of a two-layer system. As the result, at \(\sigma_1 = \sigma_2\) the antiferromagnetic order parameter is oriented perpendicularly to the magnetizations of ferromagnetic layers which thus appear to be collinear (parallel or antiparallel). Such a state is termed here as \(C\)-phase.

For \(\alpha_{af}a \gg 1\) and the distance \(\delta_{af} \ll R \ll a\), the static vortices are formed in an antiferromagnetic interlayer near the interfaces. For lower values of \(R\) the system changes over to the region of small distortions.

If \(\alpha_{af}a \ll 1\), the transition from the \(B\)-phase to \(C\)-phase takes place already in the region of small distortions. Along with the \(B\)-phase, the \(C\)-phase is characterized by a presence of a wealth of metastable states. The numerical calculations has shown the \(B \rightarrow C\) phase transitions to be of the first order. Both phases coexist in the entire region of \(R\) values and their specific energies become equal at a certain value \(R^* \sim a\) (Fig. \[6\]). The phase diagram of the three-layer system is exposed in Fig. \[7\]. In the distribution of spins in a two-layer ferromagnet — layered antiferromagnet system is modeled numerically on the bases of Ising model. However, the Ising model corresponds to very strong anisotropy of easy-axis type and is invalid for the description of multilayer structures of the \(Fe/Cr\) type, for which the anisotropy energy in the plane of the layers is much lower than the exchange interaction energy. The domain walls formed within the framework of the Ising model have atomic widths, so that the unique properties of domain walls in the multilayers ferromagnet — layered antiferromagnet where not observed in the cited paper. The orientation of spins in the three-layer system has been calculated in Ref. \[19\] within the framework of a discrete model for the case \(R \sim a\), the magnetizations of ferromagnetic layers being assumed to be mutually orthogonal. The behavior of the system in the whole range of \(R\)-values has not been analyzed.

The value of \(R^*\) is independent of temperature, therefore the \(B \rightarrow C\) phase transition is not observable under changes of temperature of the system. The transition from the state with strong biquadratic coupling to the low-temperature state with a weak coupling between the layers is unrelated to the transition considered above. The transition considered in Ref. \[18\] is caused by the fact that as approaching \(T_N\), the interaction of ferromagnetic layers via the antiferromagnetic order parameter decreases and becomes equal to the interaction via spin polarization induced in the antiferromagnet (the RKKY interaction). For higher temperature the latter dominates.
VI. CONCLUSIONS

Let us state the main results and conclusions of the work exposed above.

1. It is proposed a simple model allowing one to find the distribution of spins in “ferromagnet–antiferromagnet” frustrated layered structures.

2. The “thickness–roughness” phase diagrams for a thin ferromagnetic film on antiferromagnetic substrate and for a “ferromagnet–antiferromagnet–ferromagnet” three-layer system are obtained.

3. The transition from a polydomain state to a single-domain state is continuous and, in the strict sense, is not a phase transition.

4. The transition from the phase with mutually perpendicular orientation of magnetizations of ferromagnetic layers (B-phase) to the phase with collinear magnetizations of the layers (C-phase) constitutes a true first-order phase transition.

5. The “magnetic proximity” phenomenological model proposed by Slonczewski is shown to be adequate for the B-phase only. The parameters of the model are calculated for the entire range of its applicability.

ACKNOWLEDGMENTS

This work is partly supported by Russian Foundation for Basic Research, grant 00-02-17162.

1 M. N. Baibich, J. M. Broto, A. Fert, Nguyen van Dau, F. Petroff, P. Etienne, G. Creuzet, A. Friederich, and J. Chazelas, Phys. Rev. Lett. 61, 2472 (1988).
2 A. Schreyer, C. F. Majkrzak, Th. Zeidler, T. Schmitte, P. Bodeker, K. Theis-Brohl, A. Abromeit, J. A. Dura, and T. Watanabe, Phys. Rev. Lett. 79, 4914 (1997).
3 P. Bodeker, A. Schreyer, and H. Zabel, Phys. Rev. B 59, 9408 (1999).
4 M. Chirita, G. Robins, R. L. Stamp, R. Sooryakumar, M. E. Filipkowski, C. J. Gutierrez, and G. A. Prinz, Phys. Rev. B 58, 869 (1998).
5 S. Yan, R. Schreiber, F. Voges, C. Osthower, and P. Grünberg, Phys. Rev. B 59, R11641 (1999).
6 A. I. Morosov and A. S. Sigov, Physics Solid State 41, 1130 (1999).
7 J. C. Slonczewski, J. Magn. Magn. Mater. 150, 13 (1995).
8 A. Berger and H. Hopster, Phys. Rev. Lett. 73, 193 (1994).
9 E. J. Escorcia-Aparicio, H. J. Choi, W. L. Ling, R. K. Kawakami, and Z. Q. Qiu, Phys. Rev. Lett. 81, 2144 (1998).
10 C. M. Schmidt, D. E. Bürgler, D. M. Schaller, F. Meisinger, and H. J. Güntherodt, Phys. Rev. B 60, 4158 (1999).
11 E. J. Escorcia-Aparicio, J. H. Wolfe, H. J. Choi, W. L. Ling, R. K. Kawakami, and Z. Q. Qiu, Phys. Rev. B 59, 11892 (1999).
12 M. Freyss, D. Stoeffler, and H. Dreysse, Phys. Rev. B 56, 6047 (1997).
13 V. D. Levchenko, A. I. Morosov, A. S. Sigov, and Yu. S. Sigov, J. Exp. Theor. Phys. 87, 985 (1998).
14 L. M. Kosterlitz, D. J. Thouless, J. Phys. C 6, 1181 (1973).
15 R. Arias and D. L. Mills, Phys. Rev. B 59, 11871 (1999).
16 A. I. Morosov and A. S. Sigov, Physics Solid State 39, 1104 (1997).
17 A. Berger and E. E. Fullerton, J. Magn. Magn. Mater. 165, 471 (1997).
18 C. Cornea and D. Stoeffler, Europhys. Lett. 49, 217 (2000).
19 E. E. Fullerton, C. H. Sowers, and S. D. Bader, Rev. B 56, 5468 (1997).

FIG. 1. Frustrations in the system “ferromagnet–layered antiferromagnet” caused by the presence of atomic steps on the interfaces.

FIG. 2. Dependence of the domain wall width on the distance to the interface for $\alpha_{af} a \gg 1$ ($\alpha_{af} = 1$ and $a = 32$).

FIG. 3. Domain wall in the two-layer system for $\gamma \gg 1$. Levels of order parameters $\theta_i$ in radians are shown by various hatching (see insert). The distribution was found for $\gamma = 8$, $\alpha = 1$, $a = 8$. The value $z = 0$ corresponds to the interface between the film and the substrate. Step is situated at the point $x = 0$.

FIG. 4. Static spin vortices in the film-substrate system for $\gamma \gg 1$. Levels of order parameters $\theta_i$ in radians are shown by various hatching (see insert). The distribution was found for $\gamma = 8$, $\alpha = 0.01$, $a = 8$. The value $z = 0$ corresponds to the interface between the film and the substrate. Steps are situated at the points $x = \pm 10$.

FIG. 5. Phase diagram of the two-layer system. For demonstration the lines corresponding to equations $R = \delta_f$ and $R = \delta_0^f$ are drawn.

FIG. 6. Domain wall in the three-layer system: $\alpha_{af} a \ll 1$ (a); $\alpha_{af} a \gg 1$ (b). Levels of order parameters $\theta_i$ in radians are shown by various hatching (see insert). The values $z = 0$ and $z = 16$ correspond to the interlayer interfaces. Step is situated at the point $x = 0$, $z = 0$. The distributions were found for $\gamma = 10$, $\alpha = 0.01$, $a = 16$ (a) and $\gamma = 10$, $\alpha = 1$, $a = 16$ (b). In the Fig. (c) is represented the central part of the distribution shown in the Fig. (b).
FIG. 7. Dependence of $B$- and $C$-phases specific energy on the distance $R$ between the steps ($a = 64$, $\alpha_f = 8$, $\alpha_{af} = 1$).

FIG. 8. Phase diagram of the three-layer system. For demonstration the lines corresponding to equations $R = \delta_f$, $R = a$, and $R = \delta_0^{af}$ are drawn.
Domains

Vortices

Weak distortions

$\delta a$

$(\gamma a b)^{-1}$
