Metastable noncollinear canted states from a phenomenological model of a symmetric ferromagnetic film

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In the present work we developed a theoretical method to find the noncollinear canted magnetic states of ferromagnetic film whose magnetic properties are treated within a simple phenomenological model that takes into account the discrete location of atomic layers. We apply this method to the description of stable and uniform in the film plane magnetic configurations of symmetric ferromagnetic film with equal anisotropy constants at both sides of a film. We demonstrated that besides the ground noncollinear canted state caused by the competition between the energies of surface and bulk anisotropy this film also exhibits metastable noncollinear canted states that are not necessarily caused by the competition between these energies. They represent various kinds of excited Bloch wall-like states with a wall parallel to the film plane. The generalization of the method developed to the case of explicit account of dipole interaction between the nearest-neighbor layers is presented. We considered the fcc and bcc films with (001) surface and demonstrated that novel metastable states discovered in the present work are not the artifact of a simple model of a film used. To prove this statement we demonstrate that these states exist when the dipole interaction between the nearest-neighbor layers is explicitly taken into account.

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I. INTRODUCTION

In the theoretical investigations of magnetic properties of thin ferromagnetic films a considerable attention was paid to the determination of magnetization profile across the film thickness.[1–6] These investigations were stimulated by the necessity to describe spin-reorientation transitions[7] discovered in thin Fe, Co, and Ni films with film thickness or temperature as well as by the perspective to use these films in spintronics devices.[8] In most of these works a symmetric film with equal surface anisotropy constants at both sides of the film was considered. Such a film corresponds, for example, to a Au/Co/Au sandwich.[9–11] These investigations were performed under the assumption that the magnetic state is uniform in the film plane. It was established that depending on the magnitude of the reduced anisotropy constants (referred to as $k_S=2K_S/J$ for the surface and $k_B=2K_B/J$ for the bulk, where J is the exchange interaction between atomic layers), the film can be in a stable magnetic configuration which is uniform across the film, with a perpendicular or in-plane orientation of the vector magnetization ($\perp$ and $\parallel$ states) or in *canted noncollinear* state designated here as $\angle$ state when there is competition between the surface and bulk anisotropy energies (k_S and k_B have different signs).[1–7,12,13]

In the predominant majority of works the description of stable $\angle$ states in thin films was performed within the following expression for the reduced thermodynamic potential (TP) which is the simplest model of a thin film:[1–4,6,12–14]

$$\psi(\boldsymbol{\theta})=\frac{\Psi}{J}=-\sum_{n=1}^{N-1}\cos(\theta_n-\theta_{n+1})+\frac{k_{1S}}{2}\sin^2(\theta_1)+\frac{k_B}{2}\sum_{n=2}^{N-1}\sin^2(\theta_n)+\frac{k_{NS}}{2}\sin^2(\theta_N). \qquad (1)$$

In phenomenological model, Eq. (1), $\boldsymbol{\theta}\equiv(\theta_1,\theta_2,\ldots,\theta_N)$, the energy of exchange interactions between atomic layers is assumed to be independent on the layer index $J_{n,n+1}\equiv J>0$. The magnetization of each macroscopic atomic layer, $\boldsymbol{M}_n$, is treated as classical vector whose absolute value, M, is independent on the layer index. The vector magnetizations of all atomic layers $\boldsymbol{M}_n$ belong to only one plane which is perpendicular to the film plane. The topmost ($n=1$) and the bottommost ($n=N$) atomic layers of a horizontal N-layer film are characterized by the reduced surface anisotropy constants $k_{1S}=2K_{1S}/J$ and $k_{NS}=2K_{NS}/J$ respectively. The inner atomic layers ($n=2,\ldots,N-1$) are characterized by the reduced bulk anisotropy constant $k_B=2K_B/J$. θ_n is orientation angle between the magnetization $\boldsymbol{M}_n$ of the nth atomic layer and the film plane. In the present work we investigate $\angle$ states in a symmetric film ($k_{1S}=k_{NS}\equiv k_S$) with account of discreteness of atomic layers. Such a model could correspond, for example, to an ultrathin Co film ($N\sim 10$) in a sandwich Au/Co/Au/.

So far all conventional methods to find the ground state for a given magnitudes of model parameters k_S and k_B corresponding to model (1) were based on finding the magnetization profile across the film thickness, i.e., the dependence of orientation angles θ_n on layer index n.[1–6] However the finding of magnetization profile across the film thickness with account of discrete location of atomic layers is a difficult task. The difficulty is caused mainly by the necessity to solve the following system of equations for N orientation angles θ_n obtained after the minimization of TP, Eq. (1), with respect to each θ_n:

$$n=1,\quad \frac{\partial\psi}{\partial\theta_1}=\sin(\theta_1-\theta_2)+\frac{k_S}{2}\sin(2\theta_1)=0,$$

$$2\le n\le N-1,$$

$$\frac{\partial\psi}{\partial\theta_n} = -\sin(\theta_{n-1}-\theta_n) + \sin(\theta_n-\theta_{n+1}) + \frac{k_B}{2}\sin(2\theta_n) = 0,$$

$$n = N, \quad \frac{\partial\psi}{\partial\theta_N} = -\sin(\theta_{N-1}-\theta_N) + \frac{k_S}{2}\sin(2\theta_N) = 0. \tag{2}$$

By this reason in the predominant majority of theoretical works the finding of the ground state of symmetric ferromagnetic film was performed within the continuum approach that ignores the discrete location of atomic layers.[1–4] Within this approach all sums in Eq. (1) were substituted by integrals and the orientation-angle profile was described by the function $\varphi(x)$ that depends on the continuous coordinate $x \in [0,2a]$. In these works the orientation angles are conventionally measured from the normal to the surface plane: $\varphi(x)=\pi/2-\theta(x)$. The minimization of functional $\psi[\varphi(x)]$ leads to Euler differential equation for the function $\varphi(x)$ with two boundary conditions for $\varphi(x)$ at two sides of a film. However the authors of these works solved the problem only in the first half, $x\in[0;a]$, of the whole interval, $[0;2a]$. To obtain the solution in the whole interval $[0;2a]$ they used the following symmetry argument: since the film considered is symmetric then the solution $\varphi(x)$ has to be even with respect to the middle of the film $x=a$. This intrusion of a symmetry of a film to the solution $\varphi(x)$ searched leads to the loss of a considerable part of solutions of model (1). In particular, as it will be demonstrated below, all the solutions corresponding to metastable ∠ states of symmetric film were lost in these works. However it is well known that magnetic state of a sample is determined by its history rather than only by the present conditions, i.e., long-lived metastable states are often met in magnetism.[15]

To determine the orientation-angle profile with account of discrete location of atomic layers in a film the perturbation theory was applied.[5] The deviation of orientation angles θ_n from the average magnitude of orientation angle over the whole film $\bar{\theta}$ served as the so-called small parameters of the perturbation theory. This is very laborious method and it is applicable only if k_B is very small. It allows one to describe approximately only the ground ∠ state.

Also the iterative procedure was used. Within this method one should first choose the initial spin configuration of a film and then to successively rotate vector magnetization of each atomic layer to the direction of local molecular field until the consistency is achieved.[6,16] The dependence of the resulting magnetic configuration on the initial given spin configuration is characteristic of this iterative procedure. Guessing the initial spin configuration which is equivalent to the determination of initial point in the N-dimensional space of orientation angles θ_n is a serious obstacle in the usage of this iterative procedure because the algorithm for the determination of this point is absent.

Therefore, none of the conventional methods to find and investigate ∠ states of a symmetric film described by the model (1) allows one to determine the number and the kind of stable ∠ states for a given magnitude of model parameters k_S, k_B, and N. Consequently, the application of these methods to investigation of model (1) did not allow the authors of Refs. 1–6 to discover the metastable ∠ state of a symmetric film because the solutions corresponding to these states were lost.

We realize that more realistic model of ferromagnetic film must take into account higher order anisotropy constants, dipole interactions, external magnetic field, etc. We have to stress that in the present work we use the simplest model (1) of ferromagnetic film only to present the essence of a new method to find the ∠ states of a film as clear as possible. In the last section of the present work we generalize the model (1) to the case of explicit account of dipole interactions in a film because the account of the dipole interactions requires the most substantial modification of the method developed.

The main goals of the present work are therefore the following: (a) to develop new method to find ∠ states that correspond to uniform magnetic structure in the plane of a ferromagnetic film described by the model (1) that can help one to unambiguously answer the question about the number and the kind of stable ∠ states for a given magnitude of model parameters N, k_S, and k_B (Sec. II); (b) to describe the magnetization orientation of the atomic layers corresponding to metastable ∠ states in a particular case of symmetric ferromagnetic film and to demonstrate that in contrast to the ground ∠ state the metastable ∠ states are not necessarily caused by the competition between the surface and bulk anisotropy energies (Sec. II); and (c) to generalize the method developed in the present work to the case of explicit account of dipole interaction between the nearest-neighbor layers and thus to demonstrate that novel metastable states discovered within a simple phenomenological model (1) are not the artifact of the simplicity of model (1) (Sec. III).

II. METHOD

Now let us describe the essence of new method to find a ∠ states of a film developed in the present work. It follows from Eq. (2) that if the components of a vector $\boldsymbol{\theta}$ satisfy the set of Eqs. (2) then components of vectors $-\boldsymbol{\theta}$, $\boldsymbol{\theta}+\boldsymbol{\pi}$, and $-\boldsymbol{\theta}+\boldsymbol{\pi}$ also satisfy it, $\boldsymbol{\pi}\equiv(\pi,\pi,\ldots,\pi)$. Because of that one may restrict the search of solutions of Eqs. (2) to the interval $0\le\theta_1\le\pi/2$. Note that one can express all the angles θ_n $(n=2,\ldots,N-1)$ via the single angle θ_1 using one after another the first $(N-1)$ equations in Eqs. (2)

$$n = 2, \quad \theta_2(\theta_1) = \theta_1 + \arcsin\left[\frac{k_S}{2}\sin(2\theta_1)\right],$$

$$3 \le n \le N, \tag{3}$$

$$\theta_n(\theta_1) = \theta_{n-1}(\theta_1) + \arcsin\left\{\sin[\theta_{n-1}(\theta_1)-\theta_{n-2}(\theta_1)] + \frac{k_B}{2}\sin[2\theta_{n-1}(\theta_1)]\right\}.$$

The resulting set of equations, Eqs. (3), determine a line in the N-dimensional space $[\theta_1,\theta_2(\theta_1),\ldots,\theta_N(\theta_1)]$, $\theta_1\in[0,\pi/2]$. Now let us substitute all the angles θ_n in the expression for the TP, Eq. (1), by the functions $\theta_n(\theta_1)$ [Eqs.

(3)]. Then one obtains the function $\Phi(\theta_1) \equiv \psi[\theta_1, \theta_2(\theta_1), \ldots, \theta_N(\theta_1)]$ which gives the magnitude of the TP, ψ, on the line determined by Eq. (3) in the N-dimensional space. The coordinates of all points on this line satisfy the first $(N-1)$ equations of Eqs. (2) and, therefore, it is possible to reduce the difficult problem of finding minima of the TP $\psi(\theta_1, \ldots, \theta_N)$ in the N-dimensional space to the much simpler problem of finding minima of the TP $\psi(\theta_1, \ldots, \theta_N)$ only on the line determined by the set of Eqs. (3). This is equivalent to the finding of minima of $\Phi(\theta_1)$ in the interval $\theta_1 \in [0, \pi/2]$. Note that on deriving Eqs. (3) from Eqs. (2) we did not use the very last equation in Eqs. (2). For this reason some minima of $\Phi(\theta_1)$ may appear to be not corresponding to local minima of TP $\psi(\boldsymbol{\theta})$. Indeed, since the first $(N-1)$ equations in Eqs. (2) are satisfied, i.e., $\partial\psi/\partial\theta_n=0$ for $n=1, \ldots, N-1$, the necessary condition for the function $\Phi(\theta_1)$ to be minimal can be written as

$$\frac{d\Phi(\theta_1)}{d\theta_1} = \frac{\partial\psi}{\partial\theta_1} + \sum_{n=2}^{N} \frac{\partial\psi}{\partial\theta_n}\frac{d\theta_n}{d\theta_1} = \frac{\partial\psi}{\partial\theta_N}\frac{d\theta_N}{d\theta_1}. \tag{4}$$

Evidently, the satisfaction of condition (4) corresponds to the necessary condition for the TP, ψ, to be minimal only if it is provided by the equality $\partial\psi/\partial\theta_N=0$. However if $\partial\psi/\partial\theta_N \neq 0$, then the satisfaction of condition (4) can be provided by the satisfaction of equality $d\theta_N/d\theta_1=0$. Such a minimum of the function $\Phi(\theta_1)$ does not correspond to the necessary condition for the TP to be minimal, as $\partial\psi/\partial\theta_N \neq 0$.

We need to select such minima of $\Phi(\theta_1)$ that do correspond to the local minima of TP $\psi(\boldsymbol{\theta})$, i.e., to stable states of a film. Bearing in mind the specificity of interrelation between the minima of $\Phi(\theta_1)$ and the local minima of TP $\psi(\boldsymbol{\theta})$ mentioned above one should realize that each minimum of $\Phi(\theta_1)$ is a subject for the special investigation. First, one should find the position of each local minimum $\theta_1^{(0)}$ of the function $\Phi(\theta_1)$ in the interval $\theta_1 \in [0, \pi/2]$ by means of any conventional numerical method. Then one should determine which of them are provided by the equality $d\theta_N/d\theta_1=0$ and which ones by $\partial\psi/\partial\theta_N=0$. The simplest way to do this is to determine the roots of a function that figures in the left part of the last equation in a set of Eqs. (2) where angles θ_{N-1}, θ_N are expressed via the first orientation angle θ_1. Then all the magnitudes of the angle $\theta_1^{(0)}$ that satisfy this equation will satisfy the necessary conditions $d\Phi(\theta_1)/d\theta_1=0$ and $d\theta_N/d\theta_1 \neq 0$. The minima corresponding to the magnitude of θ_1 provided by the equality $d\theta_N/d\theta_1=0$ are discarded. For each of the remaining minima, $\theta_1^{(0)}$, one should find the orientation angles $\theta_2^{(0)}, \ldots, \theta_N^{(0)}$ with the help of the chain of equations in Eqs. (3). Then one has to find whether or not the set of angles $\boldsymbol{\theta}^{(0)} \equiv (\theta_1^{(0)}, \theta_2^{(0)}, \ldots, \theta_N^{(0)})$ corresponds to stable state of a film. To do that one should expand the TP at the point $\boldsymbol{\theta}^{(0)}$ in series up to the quadratic terms. If the obtained quadratic form is positive definite then the TP has local minimum at point $\boldsymbol{\theta}^{(0)}$ and, thus, it is stable state. In the present work to determine the sign of the quadratic form we calculated all the eigenvalue of the matrix $A_{mn} \equiv \partial^2\psi/\partial\theta_m\partial\theta_n$ corresponding to this quadratic form obtained at the point $\boldsymbol{\theta}^{(0)}$. If all the eigenvalue are positive then the quadratic form is positive definite and, thus, the set of angles $\boldsymbol{\theta}^{(0)}$ corresponds to stable state of a film. Even if only one eigenvalue is negative such a set $\boldsymbol{\theta}^{(0)}$ corresponds to unstable state.

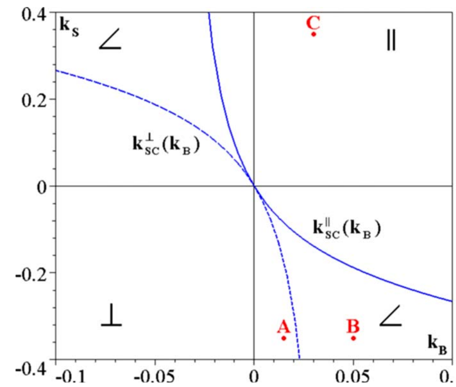

FIG. 1. (Color online) The (k_B, k_S) diagram of the ground magnetic states of the N-layer symmetric ferromagnetic film, $N=17$. Blue solid line $k_{SC}^{\parallel}(k_B)$ determines the border between the $\angle$ and $\parallel$ regions. Blue dashed line $k_{SC}^{\perp}(k_B)$ determines the border between the $\angle$ and $\perp$ regions.

To demonstrate the efficiency of this method applied here for the finding stable $\angle$ states in a symmetric ferromagnetic film it is desirable to have the (k_B, k_S) diagram of the ground magnetic states of this film for any magnitude of film thickness, N. One can show that analytic expressions for the criteria of stability of $\perp$ and $\parallel$ states of a symmetric film considered here can be obtained from a similar analytic expressions for the criteria of stability of $\perp$ and $\parallel$ states of a bare film, $k_{S1}=k_S$ and $k_{SN}=k_B$, by the substitution $N \to 2N$. The criteria of stability of $\perp$ and $\parallel$ states of a bare film are presented in Appendices A and B in Ref. 13. Based on these criteria it is possible to construct the (k_B, k_S) diagram of the ground magnetic states of symmetric film. This diagram for $N=17$ is presented in Fig. 1. In the present work we only consider films with fcc and bcc crystal structure and (001) face, z axis is perpendicular to the film surface. It is well known that bulk cubic lattices do not exhibit second-order anisotropy. Because of that here for the sake of simplicity we believe that bulk anisotropy energy, which is characterized by the reduced anisotropy constant, k_B, is provided by the magnetostatic anisotropy that originates from the dipole interaction inside each atomic layer. The effect of dipole interaction between atomic layers will be considered in Sec. III. Bearing this in mind here we consider only right part of the (k_B, k_S) diagram in Fig. 1, i.e., $k_B > 0$.

The plots $\Phi(\theta_1)$ versus $\theta_1 \in [0, \pi/2]$ for the $A(k_B=0.015,\ k_S=-0.35)$, $B(k_B=0.05,\ k_S=-0.35)$, and $C(k_B=0.03,\ k_S=0.35)$ points located in the $\perp$, $\angle$, and $\parallel$ regions in the (k_B, k_S) diagram (Fig. 1) are presented in Figs. 2(a)–2(c), respectively. In this figure the minima of the function $\Phi(\theta_1)$ corresponding to stable (unstable) states are marked by black (void) circles.

One can see that $\Phi(\theta_1)$ plotted for the point A, has three minima [Fig. 2(a)]. As expected the global minimum of $\Phi(\theta_1)$ at $\theta_1=\pi/2$ corresponds to the stable ground $\perp$ state because point A is located in the $\perp$ region in the (k_B, k_S) diagram. Also one can see that $\Phi(\theta_1)$ has a minimum at $\theta_1 \approx 1.043$ that corresponds to a stable $\angle$ state designated as a

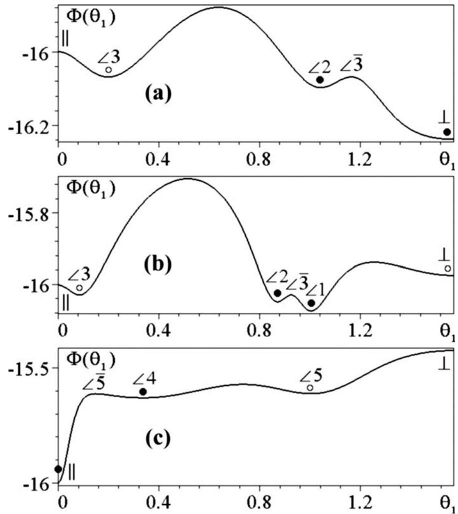

FIG. 2. [(a)–(c)] Plots of function Φ versus $\theta_1 \in [0,\pi/2]$ for the points A, B, and C, located in the $\perp$, $\angle$, and $\parallel$ regions in the (k_B,k_S) diagram, respectively (Fig. 1). The stable (unstable) states are marked by black (void) circles.

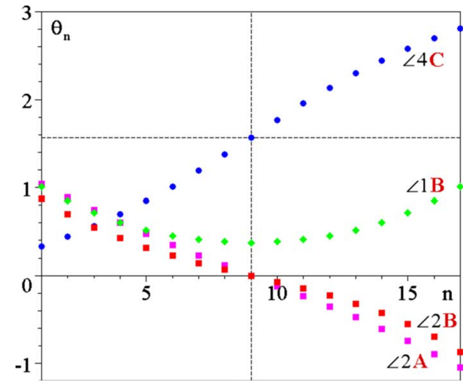

FIG. 4. (Color online) Plots of orientation angles θ_n (radians) versus layer index $n=1,\ldots,17$ for various $\angle$ states obtained for the A, B, and C points shown in the (k_B,k_S) diagram (Fig. 1): (a) green diamonds correspond to the ground $\angle 1$ state obtained for the point B, (b) red boxes correspond to metastable $\angle 2$ state obtained for the point B, (c) magenta boxes correspond to metastable $\angle 2$ state obtained for the point A, and (d) blue circles correspond to metastable $\angle 4$ state obtained for the point C.

$\angle 2$ state. However the magnitude of TP corresponding to the $\angle 2$ state is higher than the magnitude of TP corresponding to the ground $\perp$ state. Therefore, the $\angle 2$ state is a metastable state of a film. The schematic of magnetic configuration corresponding to $\angle 2$ state is presented in Fig. 3. The plot of orientation angle, θ_n, versus atomic layer index, n, for the $\angle 2$ state obtained for the point A is presented in Fig. 4. One can see that the metastable $\angle 2$ state corresponds to an odd dependence of θ_n on layer index n with respect to the middle of the film. Minimum of $\Phi(\theta_1)$ at $\theta_1 \approx 0.199$ corresponds to an unstable $\angle$ state designated as $\angle 3$ state.

One can see that $\Phi(\theta_1)$, plotted for the point B, has four minima [Fig. 2(b)]. As expected the global minimum of $\Phi(\theta_1)$ at $\theta_1 \approx 1.005$ corresponds to the stable ground $\angle$ state designated as the $\angle 1$ state because point B is located in the $\angle$ region in the (k_B,k_S) diagram. The schematic of magnetic configuration corresponding to the $\angle 1$ state is presented in Fig. 3. The plot of orientation angle, θ_n, versus layer index, n, for the $\angle 1$ state (Fig. 4) demonstrates that the ground $\angle 1$ state has an even n dependence of θ_n with respect to the middle of the film. One can show that when point B approaches the $\angle-\parallel$ border the $\angle 1$ state continuously transforms into the $\parallel$ state. Similarly, when the point B approaches the $\angle-\perp$ border the $\angle 1$ state continuously transforms into the $\perp$ state. $\Phi(\theta_1)$ has also a minimum at $\theta_1 \approx 0.872$ that corresponds to a stable $\angle 2$ state [Fig. 2(b)]. As the magnitude of the TP corresponding to $\angle 2$ state is higher than that of the ground $\angle 1$ state, the $\angle 2$ state appears to be a metastable state of the film. The schematic of magnetic configuration corresponding to the $\angle 2$ state is presented in Fig. 3. The plot of orientation angle, θ_n, versus atomic layer index, n, for the $\angle 2$ state obtained for the point B is presented in Fig. 4. The minima of $\Phi(\theta_1)$ at $\theta_1 \approx 0.085$ and $\theta_1 = \pi/2$ correspond to a $\angle 3$ state and the $\perp$ state, respectively. Both of them are unstable.

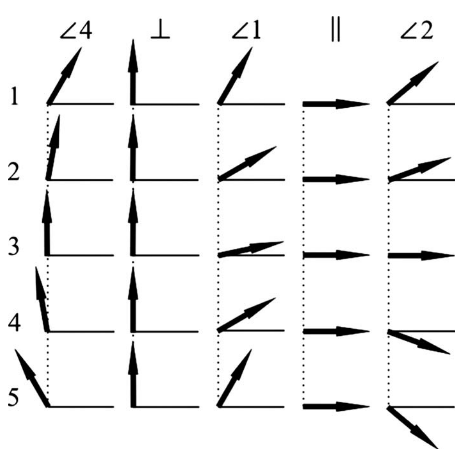

FIG. 3. The schematic of magnetic configurations corresponding to various stable states of symmetric ferromagnetic film.

One can see that $\Phi(\theta_1)$, plotted for the point C, has three minima [Fig. 2(c)]. As expected the global minimum of $\Phi(\theta_1)$ at $\theta_1=0$ corresponds to the stable ground $\parallel$ state because point C is located in the $\parallel$ region in the (k_B,k_S) diagram. Minimum of $\Phi(\theta_1)$ at $\theta_1=0.334$ corresponds to stable $\angle$ state designated as $\angle 4$ state. As the magnitude of the TP corresponding to $\angle 4$ state is higher that of the ground $\parallel$ state the $\angle 4$ state appears to be a metastable state of the film. The schematic of magnetic configuration corresponding to the $\angle 4$ state is presented in Fig. 3. The plot of orientation angle, θ_n, versus the atomic layer index n for the $\angle 4$ state obtained for the point C is presented in Fig. 4. One can see that the $\angle 4$ state corresponds to the odd dependence of orientation angles, $\alpha_n = \pi/2 - \theta_n$, on the atomic layer index, n with respect to the middle of a film. Minimum of $\Phi(\theta_1)$ at $\theta_1 \approx 1.004$ in Fig. 2(c) corresponds to an unstable $\angle$ state designated as $\angle 5$ state.

In Figs. 2(a) and 2(b) maximums that separate $\angle 2$ and $\perp$ ($\angle 1$) states correspond to states designated as $\angle\bar{3}$ state. The $\angle\bar{3}$ state is a true extremum of TP $\psi(\boldsymbol{\theta})$. In case of symmetric film this state is physically equivalent to $\angle 3$ state. Indeed

the orientation angular profile corresponding to $\angle\bar{3}$ state can be obtained from the orientation angular profile corresponding to $\angle 3$ state by means of reflection with respect to a plane which is a middle of a film. Consequently both $\angle\bar{3}$ and $\angle 3$ states have the same energy and the matrixes $A_{mn} \equiv \partial^2\psi/\partial\theta_m\partial\theta_n$ corresponding to these states have the same set of eigenvalue. One of these eigenvalue is negative.

States $\angle 3$ and $\angle\bar{3}$ correspond to saddle points in the $(N+1)$-dimensional space $(\theta_1,\theta_2,\ldots,\theta_N,\Psi)$. The results of our additional investigation, performed by means of numerical calculations, have shown the following. The $\angle\bar{3}$ state is a barrier state that separates stable $\angle 2$ state and $\perp(\angle 1)$ state [Figs. 2(a) and 2(b)]. The $\angle 3$ state is a barrier state for a stable state $\angle 2$ and the other stable state that can be obtained from the $\perp(\angle 1)$ state with the help of the following substitution $\theta_n \to -\theta_n$. Note that in the beginning of Sec. II we had already mentioned that besides the extremum states in the interval $0 \le \theta_1 \le \pi/2$ there also exist extremum states obtained by means of the substitution $\theta_n \to -\theta_n$. Similar situation takes place for $\angle 5$ and $\angle\bar{5}$ states [Fig. 2(c)]. The $\angle\bar{5}$ state is a barrier state that separates $\angle 4$ and $\|$ states. The rest maximums which are not marked in Fig. 2 [one maximum in Figs. 2(a) and 2(c) and two maximums in Fig. 2(b)] are not true maximums TP $\psi(\boldsymbol{\theta})$ because they are provided by the equality $d\theta_N/d\theta_1=0$.

It follows from the (k_B,k_S) diagram (Fig. 1) that the $\angle$ region corresponding to the ground $\angle$ state is located in the second and fourth quadrants where k_B and k_S have different signs. This means that the ground $\angle 1$ state [Fig. 2(b)] can be realized only in case of a competition between the surface and bulk anisotropy energies of a film. In contrast to this the realization of the $\angle 4$ state is not caused by the competition between the surface and bulk anisotropy energies. Indeed the $\angle 4$ state was found for the point C located in the first quadrant in the (k_B,k_S) diagram (Fig. 1) where both $k_B > 0$ and $k_S > 0$. This should not come as a surprise because metastable $\angle 4$ state is a *part of a bulklike Bloch wall* (Fig. 4), i.e., it is an excited state of a symmetric film. We remind the reader that a Bloch wall in a bulk samples is an excited state too. Indeed one can get convinced that for the $\angle 4$ state in the limiting case $N \to \infty$ the orientation angles θ_1 and θ_N approach 0 and π, respectively. At the same time the most considerable change in orientation angles with layer index takes place in the central part of a film. It is this magnetic configuration that is typical for the Bloch wall in the bulk sample.

The metastable $\angle 2$ state is an excited metastable state of a film too. It is a characteristic of magnetic configuration corresponding to the $\angle 2$ state (Fig. 3) that if the film thickness is larger than the bulklike Bloch wall then the most considerable change in orientation angles, θ_n, with layer index, n, takes place in the surface regions of a film. Such a behavior of θ_n with n for the $\angle 2$ state is caused by the competition between the surface and bulk anisotropy energies. Note that $\angle 2$ state is found for the points A and B located in the region where $k_B > 0$, $k_S < 0$. It is this reason for the difference between the kinds of magnetic configurations corresponding to $\angle 2$ and $\angle 4$ states is more distinct with film thickness N. Therefore, in the absence of competition between the surface and bulk anisotropy energies (k_B and k_S have the same sign) the most considerable change in orientation angles takes place in the central part of a film ($\angle 4$ state). In contrast to this, in case of a competition between these energies (k_B and k_S have different signs) the most considerable change in orientation angles, θ_n, with layer index takes place in the surface regions of a film ($\angle 2$ state).

III. ACCOUNT OF THE DIPOLE INTERACTION BETWEEN LAYERS

One can add terms corresponding to the fourth-order anisotropy constant to the model (1). Also one can take into account terms corresponding to the interaction with external magnetic field. The most significant modification of the method developed in Sec. II is required to account the dipole interaction between atomic layers. In the present section we restrict our consideration only by investigation of films with cubic lattices and (001) face parallel to the film surface. The most considerable contribution to magnetostatic energy of a film is made by the terms included in TP, Eq. (1), that describe the dipole interaction inside the atomic layers. In this case the reduced bulk anisotropy constant k_B can be written as

$$k_B = \frac{\mu_0}{4\pi}\frac{3S_0 m^2}{2a^3 J}. \tag{5}$$

We imply that the same contribution is included in k_S. In Eq. (5) μ_0 is permeability of vacuum, m is magnetic moment per one site of a lattice, a is a lattice parameter, and S_0 is a two-dimensional lattice sum

$$S_0 = \sum_{r_i \neq 0}\frac{1}{r_i^3},$$

where the distances between sites, r_i, are measured in units of a lattice parameter a.

Also the terms describing the dipole interaction between atomic layers make a substantial contribution to the magnetostatic energy of a film. This contribution to TP, Eq. (1), can be written as

$$\Delta\psi_{d\text{-}d} = g\sum_{n=1}^{N-1}[\cos(\theta_n - \theta_{n+1}) - 3\cos(\theta_n + \theta_{n+1})], \tag{6}$$

where we introduced the dipole interaction constant, g, which can be expressed via k_B

$$g = \eta k_B; \quad \eta = \frac{S_1}{6S_0}. \tag{7}$$

Here we introduced two-dimensional sum

$$S_1 = \sum_{r_i \neq 0}\left[\frac{1}{r_i^3} - \frac{3d_i^2}{r_i^5}\right],$$

where d_1 is a distance between atomic layers in unites of a. In the second formula in Eq. (7) the ratio of lattice sums is equal to the ratio Φ_1/Φ_0, presented in Ref. 5. For cubic lattices the parameter η is equal to

$$\eta = 0.02637 \text{ (fcc)}, \quad \eta = 0.07705 \text{ (bcc)}.$$

The magnitude of the whole magnetostatic energy per one atomic layer is presented in Ref. 17. The error in the magnitude of the whole magnetostatic energy caused by the neglecting the dipole interaction between atomic layers beyond the nearest-neighbor layers is only 0.3% for the fcc(001) lattice and 3.8% for the bcc(001) lattice. Since the magnitude of magnetostatic energy itself is a small part of the exchange interaction energy the effect of dipole interaction between atomic layers beyond the nearest-neighbor layers can be neglected with good accuracy.

Therefore, to take into account the dipole interaction between atomic layers one should only to add the correction in Eq. (6) to TP, Eq. (1). Hence the modified TP can be written in the following form:

$$\psi = \frac{k_{S1}}{2}\sin^2(\theta_1) + \frac{k_{SN}}{2}\sin^2(\theta_N) + \frac{k_B}{2}\sum_{n=2}^{N-1}\sin^2(\theta_n) + \sum_{n=1}^{N-1}[(g-1)\cos(\theta_n - \theta_{n+1}) - 3g\cos(\theta_n + \theta_{n+1})]. \quad (8)$$

Now let us introduce new (fictitious) orientation angles Θ_n whose sine and cosine are determined by the following relations:

$$\sin(\Theta_n) = (1+2g)\frac{\sin(\theta_n)}{Sq(\theta_n)},$$

$$\cos(\Theta_n) = (1-4g)\frac{\cos(\theta_n)}{Sq(\theta_n)},$$

$$Sq(\theta_n) = \sqrt{(1+2g)^2\sin^2(\theta_n) + (1-4g)^2\cos^2(\theta_n)}. \quad (9)$$

Since for the fcc(001) lattice and the bcc(001) lattices $\eta > 0$ then the parameter g in Eq. (7) is positive too. By this reason the sine of old and new angles have the same sign. We assume that old orientation angles belong to an interval $-\pi < \theta_n \le \pi$. Then new orientation angles can be defined in accordance with the following rules:

$$\Theta_n = \arccos\left[(1-4g)\frac{\cos(\theta_n)}{Sq(\theta_n)}\right], \quad \sin(\theta_n) \ge 0,$$

$$\Theta_n = -\arccos\left[(1-4g)\frac{\cos(\theta_n)}{Sq(\theta_n)}\right], \quad \sin(\theta_n) < 0. \quad (10)$$

The equilibrium conditions for TP, Eq. (8), with account of definitions in Eq. (9) can be written in the following form:

$$n=1, \quad \frac{k_{S1}}{2}\frac{\sin(2\theta_1)}{Sq(\theta_1)} + \sin(\Theta_1 - \theta_2) = 0,$$

$$1 < n < N,$$

$$\frac{k_B}{2}\frac{\sin(2\theta_n)}{Sq(\theta_n)} + \sin(\Theta_n - \theta_{n-1}) + \sin(\Theta_n - \theta_{n+1}) = 0,$$

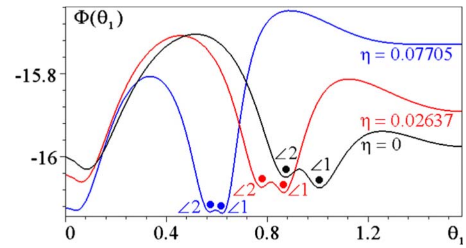

FIG. 5. (Color online) Plots of function Φ versus $\theta_1 \in [0, \pi/2]$ for the point B for the different values of parameter η: (a) black line corresponds to $\eta=0$ (without account of the dipole interlayer interaction), (b) red line corresponds to $\eta=0.02637$ [with account of the dipole interlayer interaction for fcc(001)], and (c) blue line corresponds to $\eta=0.07705$ [with account of the dipole interlayer interaction for bcc(001)].

$$n=N, \quad \frac{k_{SN}}{2}\frac{\sin(2\theta_N)}{Sq(\theta_N)} + \sin(\Theta_N - \theta_{N-1}) = 0. \quad (11)$$

Similar to the procedure presented in Sec. II all orientation angles can be expressed via the first orientation angle using one after another the first $(N-1)$ equations in Eq. (11). Indeed

$$n=2, \quad \theta_2 = \Theta_1 + \arcsin\left[\frac{k_{S1}}{2}\frac{\sin(2\theta_1)}{Sq(\theta_1)}\right],$$

$$n > 2,$$

$$\theta_n = \Theta_{n-1} + \arcsin\left[\frac{k_B}{2}\frac{\sin(2\theta_{n-1})}{Sq(\theta_{n-1})} + \sin(\Theta_{n-1} - \theta_{n-2})\right]. \quad (12)$$

Again similar to Sec. II the last equation in Eq. (11) is not used. The substitution of orientation angles θ_n determined by Eq. (12) in TP, Eq. (8), with account of definitions in Eqs. (10) gives rise to the formation of a function $\Phi(\theta_1)$ that is similar to the function $\Phi(\theta_1)$ obtained in Sec. II for the model (1).

Three plots of function $\Phi(\theta_1)$ for the point $B(k_B=0.05, k_S=-0.35)$ are presented in Fig. 5. The first plot (black line) is obtained for the case when the dipole interaction between layers is neglected, $\eta=0$. The second plot (red line) is obtained for the case when the dipole interaction between the nearest-neighbor layers is taken into account for the fcc(001) lattice, $\eta=0.02637$. The third plot (blue line) is obtained for the case when the dipole interaction between the nearest-neighbor layers is taken into account for the bcc(001) lattice $\eta=0.07705$. It follows from this figure that the account of dipole interaction tends to suppress the noncollinear state of ferromagnetic film. This effect is the most noticeable for the bcc(001) lattice. Such a behavior takes place because the effect of dipole interaction, Eq. (6) leads to appearance of effective anisotropic exchange interaction described by the following constants:

$$j_{\parallel} = 1 + 2g, \quad j_{\perp} = 1 - 4g. \tag{13}$$

Indeed, the expression in rectangular brackets in Eq. (8) can be written as

$$-(1+2g)\cos(\theta_n)\cos(\theta_{n+1}) - (1-4g)\sin(\theta_n)\sin(\theta_{n+1}).$$

Equations (13) follows from this formula. Since for the lattices considered $g > 0$ then it follows from Eq. (13) that the dipole interaction between layers favors the stabilization of $\parallel$ state and the destabilization of $\perp$ state. Because of that a partial suppression of noncollinear $\angle 1$ and $\angle 2$ states takes place. Consequently, the magnitude of equilibrium angle θ_1 is decreased for each of these states and also the energy barrier between them is decreased too.

Therefore, we have shown that method to find and to describe $\angle$ states of symmetric film developed in the present work is applicable to the model where the dipole interaction between the nearest-neighbor layers is explicitly taken in account. Also we have shown that metastable $\angle$ states discovered within a simple model of symmetric film, Eq. (1), are not the artifact of this model (1). Namely, the metastable $\angle$ states discovered also take place when the dipole interaction between nearest-neighbor layers is explicitly taken into account.

IV. CONCLUSION

In the present work we developed a theoretical method to find the noncollinear canted magnetic states of ferromagnetic film whose magnetic properties are treated within a simple phenomenological model that takes into account the discrete location of atomic layers. We apply this method to the description of stable and uniform in the film plane magnetic configurations of symmetric ferromagnetic film with equal anisotropy constants at both sides of a film. We demonstrated that besides the ground noncollinear canted state caused by the competition between the energies of surface and bulk anisotropy this film also exhibits metastable noncollinear canted states that are not necessarily caused by the competition between these energies. They represent various kinds of excited Bloch wall-like states with a wall parallel to the film plane. The generalization of the method developed to the case of explicit account of dipole interactions between the nearest-neighbor layers is presented. We considered the fcc and bcc films with (001) surface and demonstrated that novel metastable states discovered in the present work are not the artifact of a simple model of a film used. To prove this statement we demonstrate that these states exist when the dipole interaction between the nearest-neighbor layers is explicitly taken into account.

We have to note that the method to find stable $\angle$ states developed in the present work does not require laborious formula manipulation or application of complicated numerical methods. The important advantage of this method is that for a given magnitudes of model parameters N, k_B, and k_S minima of the function $\Phi(\theta_1)$ show all possible magnetic configurations of ferromagnetic film. From the other side the range of application of this method has some restrictions. For example, the first Eq. (2) allows one to express θ_2 via θ_1 in the whole interval $\theta_1 \in [0, \pi/2]$ only if the condition $|k_S| \leq 2$ is satisfied. Also there are some restrictions for the magnitude of k_B for a given magnitudes of model parameters k_S and N. At present the solution of this problem is under the consideration.

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