

BAND MODEL OF DOMAIN STRUCTURE IN FERROMAGNETIC THIN FILMS*

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The purpose of this study is to formulate the band model of ferromagnetism in a form permitting the description of domain structure in ferromagnetic thin films. The results obtained from the band model approach are in qualitative agreement with those given by classical theories, for the domain and domain wall width. However, the present approach also allows to investigate the influence of new factors connected with the band character on domain wall properties. Calculations using the band model lead to relations between microscopic and phenomenological constants characterizing the domain structure.

1. Introduction

Until recently there did not exist any general theory of domains which would give a complete distribution of magnetization inside a sample. It was possible only to calculate parameters of domain structure assuming its shape based on experimental indications. The parameters of such a structure have been calculated mainly by methods based on the minimizing of the phenomenological energy of a crystal [1]. Recently, some attempts at general formulation of the theory of domain structure were made on the basis of conformal mapping [2]. On the other hand, the theory of domain structure for the Heisenberg model of ferromagnetism has been derived by means of two methods: 1. by minimizing of the energy considered as the average value of the Heisenberg Hamiltonian in a class of especially chosen states [3], and 2. by treating the ferromagnetic state with domain structure as a state with the minimal free energy obtained by the second quanti-

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zation method [4]. Recently, the distribution of magnetization directions in ferromagnetic domain walls was also obtained from the itinerant electron model of ferromagnetism [5, 6].

The aim of this paper is to present a simplified formulation of the band model of ferromagnetism in a form permitting the description of the domain structure of a sample at zero absolute temperature and to apply this formulation to thin films. From the experimental point of view as well as from the theoretical considerations, uniaxial monocrystalline ferromagnetic thin films are the most convenient samples for investigations of domain properties. Therefore, the aim of the considerations of this paper is to describe domain structure in thin films. As a result of our theory, the parameters characterizing the domain structure are obtained in terms of the band theory. In this manner, the relations between microscopic and phenomenological constants are found.

2. The Hamiltonian

We assume that in the band model of ferromagnetism the Hamiltonian of a ferromagnetic sample with domains contains three parts: the one-band Hubbard Hamiltonian the magnetic dipolar term, and the term responsible for the anisotropy effects.

1. The one-band Hubbard Hamiltonian applied to thin films [7] is of the form

$$\mathcal{H}_{\text{Hubb}} = \sum_m \sum_{\langle vjv'j' \rangle} H \begin{pmatrix} v'j' \\ vj \end{pmatrix} c_{vjm}^+ c_{v'j'm}^- + I \sum_{vj} c_{vj\uparrow}^+ c_{vj\uparrow}^- c_{vj\downarrow}^+ c_{vj\downarrow}^-, \quad (1)$$

where c_{vjm}^{\pm} denote respectively the creation and annihilation operators for an electron with the spin $m = \uparrow(\downarrow)$ at the point j in the layer v of the film. I is the intra-atomic Coulomb integral and the coefficients $H \begin{pmatrix} v'j' \\ vj \end{pmatrix}$, determined in [8], are related to the matrix elements of the electronic potential in the Wannier representation. The sum over $\langle vjv'j' \rangle$ is limited to the nearest neighbour lattice sites only.

2. Usually the new operators S_{vj}^x , S_{vj}^y , S_{vj}^z , are introduced by means of the relations

$$\begin{aligned} S_{vj}^x &= \frac{1}{2} (c_{vj\uparrow}^+ c_{vj\downarrow}^- + c_{vj\downarrow}^+ c_{vj\uparrow}^-), \\ S_{vj}^y &= \frac{i}{2} (c_{vj\downarrow}^+ c_{vj\uparrow}^- - c_{vj\uparrow}^+ c_{vj\downarrow}^-), \\ S_{vj}^z &= \frac{1}{2} (c_{vj\uparrow}^+ c_{vj\uparrow}^- - c_{vj\downarrow}^+ c_{vj\downarrow}^-). \end{aligned} \quad (2)$$

The operators S_{vj}^{α} ($\alpha = x, y, z$) satisfy the commutation rules characteristic for spin operators. Thus, we can interpret them as the operators of the spin at the point (vj) . In terms of these operators we can introduce the part of the Hamiltonian corresponding to the magnetic dipolar interactions of electrons [9] by the formula:

$$\begin{aligned} \mathcal{H}_m &= \frac{1}{2} (g\beta)^2 \iint d^3r d^3r' \frac{1}{|\vec{r} - \vec{r}'|} \mathcal{S}(\vec{r}', \vec{r}) \\ \mathcal{S}(\vec{r}', \vec{r}) &= \vec{S}(\vec{r}') \vec{S}(\vec{r}) - 3 \frac{[\vec{S}(\vec{r}') \cdot (\vec{r}' - \vec{r})] [\vec{S}(\vec{r}) \cdot (\vec{r}' - \vec{r})]}{|\vec{r}' - \vec{r}|^2}, \end{aligned} \quad (3)$$

where g is the gyromagnetic factor and β denotes the Bohr magneton. Here, the relation

$$\vec{S}(\vec{r}) = \sum_{vj} \vec{S}_{vj} \varrho(\vec{r} - \vec{r}_{vj}), \quad (4)$$

between the magnetization operator $\vec{M} = g\beta\vec{S}$ at the point \vec{r} , the spin operator \vec{S}_{vj} given by (2), and the density of electrons $\varrho(\vec{r} - \vec{r}_{vj})$ centered at the point (vj) , is assumed. Then, we can rewrite formula (3) in the form

$$\mathcal{H}_m = \frac{1}{2} (g\beta)^2 \sum_{\alpha\beta} \sum_{vjv'j'} N_{vjv'j'}^{\alpha\beta} S_{vj}^{\alpha} S_{v'j'}^{\beta}, \quad (5)$$

where

$$N_{vjv'j'}^{\alpha\beta} = \iint d^3r d^3r' \left\{ \varrho(\vec{r} - \vec{r}_{vj}) \varrho(\vec{r}' - \vec{r}_{v'j'}) \nabla_r^{\alpha} \nabla_{r'}^{\beta} \frac{1}{|\vec{r} - \vec{r}'|} \right\} \quad (6)$$

denotes coefficients dependent on the geometry of a sample and on the density of electrons contributing the magnetic moment.

3. We assume the anisotropy term of the Hamiltonian in the following form

$$\mathcal{H}_{\text{anis}} = -K \sum_{vj} \langle S_{vj}^z \rangle S_{vj}^z, \quad (7)$$

where K is the parameter describing the uniaxial anisotropy energy and $\langle S_{vj}^z \rangle$ denotes the average value of S_{vj}^z taken in the ground state of the sample.

We must realize that the real anisotropy results from various physical causes (e.g. spin-orbit coupling); however, instead of considering these causes, it is sufficient for our purposes to assume that the part of the Hamiltonian responsible for anisotropy is in the form of expression (7). This kind of anisotropy term plays, as we will see in Section 4, just the same role as an uniaxial anisotropy with the easy magnetization axis directed along the z -axis [10], and it is formally equivalent to the term which was introduced into the band model by the molecular field approximation of the isotropic Hubbard Hamiltonian [11]. The relation between the parameter K and the microscopic causes will be the subject of a forthcoming paper.

In this manner, we take as a starting point of our paper the Hamiltonian which consists of the hopping term, the intraatomic Coulomb interaction term, the term corresponding to the magnetic dipolar interactions and the term responsible for the uniaxial anisotropy, namely

$$\begin{aligned} \mathcal{H} = & \sum_{m \langle vjv'j' \rangle} H \begin{pmatrix} v'j' \\ vj \end{pmatrix} c_{vjm}^+ c_{v'j'm}^- + I \sum_{vj} c_{vj\uparrow}^+ c_{vj\downarrow}^- c_{vj\downarrow}^+ c_{vj\uparrow}^- \\ & + \frac{1}{2} (g\beta)^2 \sum_{\alpha,\beta} \sum_{vjv'j'} N_{vjv'j'}^{\alpha\beta} S_{vj}^{\alpha} S_{v'j'}^{\beta} - K \sum_{vj} \langle S_{vj}^z \rangle S_{vj}^z. \end{aligned} \quad (8)$$

3. Domain structure

We consider an uniaxial thin film with its easy magnetization axis lying in the film plane. If the uniaxial anisotropy is large enough, as is assumed in the following, we can expect that domains have the form of magnetized stripes parallel and antiparallel to the easy magnetization axis and they are separated by 180° Néel or Bloch walls. For smaller anisotropy the so-called closure domains can appear; we neglect this possibility. The domain structure is considered as a one-dimensional screw structure in which the magnetization at the point (vj) is rotated by an angle ϑ_{vj} depending on one variable only. The axis of this rotation depends on the type of walls. For the Néel walls the rotation axis is perpendicular to the film plane and for the Bloch walls — it is perpendicular to the plane of walls. We assume a coordinate system in which the z — axis is directed along the easy magnetization axis of the film and the y -axis along the rotation axis of the magnetization. Taking into account that we consider the one-dimensional walls, the angle ϑ_{vj} depends on one variable only, namely on x for the Néel walls and on y for the Bloch walls.

4. The Hamiltonian of a thin with domain structure

The Hamiltonian (8) describes the magnetic properties of uniaxial thin films magnetized homogeneously. Now, with the help of it, we construct the effective Hamiltonian of a thin, film with the domain structure assumed in the preceding chapter.

For this reason we introduce new operators b_{vjm}^\pm defined by the following relations [12]:

$$c_{vjm} = \cos \frac{\vartheta_{vj}}{2} b_{vjm} + m \sin \frac{\vartheta_{vj}}{2} b_{vj-m}, \quad (9)$$

where $m = +1$ for spin up (\uparrow) and -1 for spin down (\downarrow). The transformation (9) introduced here is equivalent to the rotation of the spin operator S_{vj}^α around the y axis, namely

$$S_{vj}^\alpha = \sum_{\alpha'} R_{vj}^{\alpha\alpha'} S_{vj}^{\alpha'}, \quad (10)$$

where the matrix of this rotation is the following

$$R_{vj} = \begin{pmatrix} \cos \vartheta_{vj} & 0 & -\sin \vartheta_{vj} \\ 0 & 1 & 0 \\ \sin \vartheta_{vj} & 0 & \cos \vartheta_{vj} \end{pmatrix}, \quad (11)$$

and $S_{vj}^{\alpha'}$ is the α' -component of a spin operator expressed by the operators b_{vjm}^\pm in the same manner as S_{vj}^α by c_{vjm}^\pm (see the formula (2)). This fact allows us to interpret the angle ϑ_{vj} as an angle between magnetization at the point (vj) and the easy magnetization axis. So, the meaning of the angle ϑ_{vj} is the same as in the phenomenological theory.

It is necessary to remember that the y -axis is perpendicular to the film surfaces for the Néel walls; then ϑ_{vj} is a function of x only and the y -axis lies in the film plane for the Bloch walls when ϑ_{vj} depends on y only.

If we introduce the local spin operators $S'_{vj}{}^\alpha$ ($\alpha = x, y, z$) defined by

$$\begin{aligned} S'_{vj}{}^x &= \frac{1}{2} (b_{vj\uparrow}^+ b_{vj\uparrow}^- + b_{vj\downarrow}^+ b_{vj\downarrow}^-), \\ S'_{vj}{}^y &= \frac{i}{2} (b_{vj\uparrow}^+ b_{vj\downarrow}^- - b_{vj\downarrow}^+ b_{vj\uparrow}^-), \\ S'_{vj}{}^z &= \frac{1}{2} (b_{vj\uparrow}^+ b_{vj\downarrow}^- - b_{vj\downarrow}^+ b_{vj\uparrow}^-), \end{aligned} \quad (12)$$

and substitute the operator c_{vjm}^\pm represented by (9) into (2), we obtain after easy calculations that

$$\begin{aligned} S_{vj}{}^x &= S_{vj}^x \cos \vartheta_{vj} + S_{vj}^z \sin \vartheta_{vj}, & S_{vj}{}^y &= S_{vj}^y, \\ S_{vj}{}^z &= S_{vj}^z \cos \vartheta_{vj} - S_{vj}^x \sin \vartheta_{vj}. \end{aligned} \quad (13)$$

Thus, the transformation (9) is equivalent to the rotation of the spin operator S_{vj}^α around the y -axis.

Now, we would like to notice that it is a well known fact that the Coulomb interaction term of the Hubbard Hamiltonian is invariant with respect to the transformation (9), namely

$$I \sum_{vj} c_{vj\uparrow}^+ c_{vj\uparrow}^- c_{vj\downarrow}^+ c_{vj\downarrow}^- = I \sum_{vj} b_{vj\uparrow}^+ b_{vj\uparrow}^- b_{vj\downarrow}^+ b_{vj\downarrow}^-, \quad (14)$$

while the term (7) can be transformed in the following way

$$\langle S_{vj}^z \rangle S_{vj}^z = \langle S_{vj}^z \rangle S_{vj}^z \cos^2 \vartheta_{vj} + \langle S_{vj}^z \rangle S_{vj}^x \cos \vartheta_{vj} \sin \vartheta_{vj}, \quad (15)$$

if we take into account that $\langle S_{vj}^x \rangle = 0$ (because $\langle S_{vj}^z \rangle = S_{vj}$). As a conclusion we can see that the formula (7) does represent uniaxial anisotropy term (as well as some other term which is irrelevant for final conclusions of this paper).

Substituting (9) and (10) into (8) we obtain the Hamiltonian of a thin film with domain structure

$$\begin{aligned} \mathcal{H} &= \sum_{\langle vj, v'j' \rangle} H \left(\begin{matrix} v'j' \\ vj \end{matrix} \right) \left\{ \left(\sum_m b_{vjm}^+ b_{v'j'm}^- \right) \cos \frac{\vartheta_{vj} - \vartheta_{v'j'}}{2} \right. \\ &\quad \left. + (b_{v'j\uparrow}^+ b_{v'j\downarrow}^- - b_{vj\uparrow}^+ b_{vj\downarrow}^-) \sin \frac{\vartheta_{v'j'} - \vartheta_{vj}}{2} \right\} \\ &+ I \sum_{vj} n_{vj\uparrow} n_{vj\downarrow} + \frac{1}{2} (g\beta)^2 \sum_{\alpha\beta} \sum_{\alpha'\beta'} \sum_{vjv'j'} N_{vjv'j'}^{\alpha\beta} R_{vj}^{\alpha\alpha'} R_{v'j'}^{\beta\beta'} S_{vj}^{\alpha'} S_{v'j'}^{\beta'} \\ &- K \sum_{vj} \langle S_{vj}^z \rangle \cos \vartheta_{vj} (S_{vj}^z \cos \vartheta_{vj} + S_{vj}^x \sin \vartheta_{vj}). \end{aligned} \quad (16)$$

Applying the molecular field approximation to the Hamiltonian (16) we obtain the effective form of the Hamiltonian of a thin film with domain structure in a form which will be used in the following Sections:

$$\begin{aligned}
 \mathcal{H} = & \sum_{\langle vjv'j' \rangle} H \left(\frac{v'j'}{vj} \right) \left\{ \left(\sum_m b_{vjm}^+ b_{v'j'm}^- \right) \cos \frac{\vartheta_{v'j'} - \vartheta_{vj}}{2} \right. \\
 & + (b_{vj_t}^+ b_{v'j_t}^- - b_{vj_t}^+ b_{v'j_t}^-) \sin \frac{\vartheta_{v'j'} - \vartheta_{vj}}{2} \left. \right\} + I \sum_{vj} [n_{vj_t} \langle n_{vj_t} \rangle + \langle n_{vj_t} \rangle n_{vj_t}] \\
 & + (g\beta)^2 \sum_{\alpha, \beta} \sum_{\alpha', \beta' = z} \sum_{vjv'j'} N_{vjv'j'}^{\alpha\beta} R_{vj}^{\alpha\alpha'} R_{v'j'}^{\beta\beta'} \langle S_{v'j'}^{z'} \rangle S_{vj}^{\alpha'} \\
 & - K \sum_{vj} \langle S_{vj}^{z'} \rangle \cos \vartheta_{vj} (S_{vj}^{z'} \cos \vartheta_{vj} + S_{vj}^{x'} \sin \vartheta_{vj}), \quad (17)
 \end{aligned}$$

where K is a parameter of the theory in its present form.

5. The average value of the Hamiltonian

We assume that the transformation

$$b_{vjm}^+ = \sum_{\tau h} T_{vj, \tau h}^m b_{\tau hm}^+ \quad (18)$$

leads to the diagonal form of the Hamiltonian (17) for the homogeneous distribution of magnetization with respect to its direction i.e. for $\vartheta_{vj} = 0$. It is a well known fact that for a bulk body the coefficients $T_{vj, \tau h}^m$ are such that the transformation (18) constitutes the Fourier transformation. In the case of thin films (considered as one domain sample) these coefficients are the following

$$T_{vj, \tau h}^m = \frac{1}{\sqrt{N}} \Gamma_{v\tau}^m e^{i h \tau y}, \quad (19)$$

where N denotes the number of atoms in a layer and $\Gamma_{v\tau}^m$ are the electron eigenfunction amplitudes on the direction perpendicular to the film [8]. Now, we assume that the transformation (19) is a good approximation also for thin films with domain structure. Then the average value of Hamiltonian (17) at the zero absolute temperature can be determined by the quantum mechanical mean value taken for the ground states $|0\rangle$ for which the eigenstates $b_{\tau hm}^+ |0\rangle$ lead to the diagonal form of the Hamiltonian. We find that

$$\begin{aligned}
 \langle \mathcal{H} \rangle = & 2I \sum_{vj} \langle n_{vj_t} \rangle \langle n_{vj_t} \rangle + (g\beta)^2 \sum_{vjv'j'} N_{vjv'j'} \langle S_{vj}^{z'} \rangle \langle S_{v'j'}^{z'} \rangle - K \sum_{vj} \langle S_{vj}^{z'} \rangle^2 \cos^2 \vartheta_{vj} \\
 & + \sum_{\langle vjv'j' \rangle} H \left(\frac{v'j'}{vj} \right) \left\{ \left(\sum_m \langle b_{vjm}^+ b_{v'j'm}^- \rangle \right) \cos \frac{\vartheta_{v'j'} - \vartheta_{vj}}{2} \right. \\
 & \left. + (\langle b_{vj_t}^+ b_{v'j_t}^- \rangle - \langle b_{vj_t}^+ b_{v'j_t}^- \rangle) \sin \frac{\vartheta_{v'j'} - \vartheta_{vj}}{2} \right\}, \quad (20)
 \end{aligned}$$

where

$$\langle b_{vjm}^+ b_{v'j'm'}^- \rangle = \sum_{\tau h} T_{vj\tau h}^m T_{v'j'\tau h}^{m'} \langle b_{\tau hm}^+ b_{\tau hm'}^- \rangle, \quad (21)$$

and

$$N_{vjv'j'} = \sum_{\alpha\beta} N_{vjv'j'}^{\alpha\beta} R_{vj}^{\alpha z} R_{v'j'}^{\beta z}. \quad (22)$$

In our approximation, given by formula (19), we have

$$\langle b_{vjm}^+ b_{v'j'm'}^- \rangle \simeq \frac{1}{N} \sum_{\tau h} e^{i\vec{h}(\vec{j}-\vec{j}')} \Gamma_{v\tau}^m \Gamma_{v'\tau}^{m'} \langle b_{\tau hm}^+ b_{\tau hm'}^- \rangle. \quad (23)$$

In the further text we consider the case of the domain structure with Bloch walls only. For the Néel walls it is sufficient to change the coordinate system, i.e. to change $x \rightleftharpoons y$. Then, the angle ϑ_{vj} depends on y only. We take into account that the change of the angle ϑ_{vj} per one lattice constant a (simple cubic crystallographic structure is assumed) is very small. Then we have

$$\cos \frac{\vartheta_{v'j'} - \vartheta_{vj}}{2} = \begin{cases} 1 - \frac{1}{8} a^2 \left(\frac{d\vartheta}{dy} \right)^2 & \text{for } v'j' = v, j \pm i_y a, \\ 1 & \text{otherwise} \end{cases} \quad (24)$$

$$\sin \frac{\vartheta_{v'j'} - \vartheta_{vj}}{2} = \begin{cases} \frac{1}{2} a \frac{d\vartheta}{dy} & \text{for } v'j' = v, j \pm i_y a \\ 0 & \text{otherwise} \end{cases} \quad (25)$$

and we can change the sum over j_y into an integral according to the formula

$$\frac{1}{N_y} \sum_{j_y} (\dots) \rightarrow \frac{1}{L_y} \int_0^{L_y} dy (\dots), \quad (26)$$

where $L_y = aN_y$ is a dimension of the film along the y axis. Then, the average value of the Hamiltonian at absolute zero is

$$\langle \mathcal{H} \rangle = \langle \mathcal{H}_0 \rangle + \frac{V}{4L_y} \int_0^{L_y} dy \mathcal{L}(\vartheta(y)),$$

$$\mathcal{L}(\vartheta(y)) = \left\{ \alpha \left(\frac{d\vartheta}{dy} \right)^2 + \alpha' \left(\frac{d\vartheta}{dy} \right) + \frac{K}{a^3} \sin^2 \vartheta + \frac{(g\beta)^2}{a^6} \sum_{j_y} N_{vjv'j'} \right\}, \quad (27)$$

where

$$\langle \mathcal{H}_0 \rangle = 2I \sum_{vj} \langle n_{vj\uparrow} \rangle \langle n_{vj\downarrow} \rangle + \sum_{\tau h\sigma} \varepsilon_{\tau h\sigma} \langle n_{\tau h\sigma} \rangle + (-KV/4a^3) \quad (28)$$

represents the part of $\langle \mathcal{H} \rangle$ which does not depend on the angle ϑ_{vj} , $V = N_x N_y N_z a^3$, and

$$\varepsilon_{\tau h m} = \frac{1}{N} \sum_{\langle vjv'j' \rangle} H \begin{pmatrix} v'j' \\ vj \end{pmatrix} e^{i\vec{h}(\vec{J}-\vec{J}')} \Gamma_{v\tau}^m \Gamma_{v'\tau}^m \quad (29)$$

$$\alpha = \frac{1}{N} \frac{B}{a} \sum_{\tau h m} \langle b_{\tau h m}^+ b_{\tau h m}^- \rangle \cos h_y a, \quad B = -H \begin{pmatrix} v, j \pm i_y a \\ v, j \end{pmatrix} \quad (30)$$

$$\alpha' = \frac{4}{N} \frac{B}{a} \sum_{\tau h} [\Gamma_{v\tau}^+ \Gamma_{v'\tau}^+ \langle b_{\tau h\uparrow}^+ b_{\tau h\downarrow}^- \rangle - \Gamma_{v\tau}^- \Gamma_{v'\tau}^- \langle b_{\tau h\uparrow}^- b_{\tau h\downarrow}^+ \rangle] \cos h_y a \quad (31)$$

$$N_{vj, v'j'} = \sum_{\alpha\beta} N_{vjv'j'}^{\alpha\beta} R_{j_y}^{\alpha z} R_{j'_y}^{\beta z} \quad (32)$$

In the further text the term with α' can be omitted since the minimalization procedure does not depend on the linear expressions with respect to the derivatives of the angle ϑ_{vj} treated as a function appearing in the functional (27).

Now, it is possible to obtain the approximate form of the average value of the Hamiltonian (27) by introducing the demagnetizing factors. Namely, treating the region of lattice points $(v'j')$ which give a significant contribution to the demagnetizing field in the lattice point (vj) as an ellipsoidal region, it is possible to assume that this field is independent of $(v'j')$ and is proportional to the magnetization at the point (vj) . In this case, the proportionality factors $N^{\alpha z}$ ($\alpha = x, y, z$) between the demagnetizing field at the point (vj) and the magnetization at this point are known as demagnetizing factors. They are defined by the equation

$$\begin{aligned} \sum_{v'j'} \left\{ \sum_{\alpha\beta} N_{vjv'j'}^{\alpha\beta} R_{j_y}^{\alpha z} R_{j'_y}^{\beta z} \right\} &= \sum_{v'j', \alpha} (R_{j_y}^{\alpha z})^2 N^{\alpha z} \\ &= N_x N_y N_z (N^{xx} \sin^2 \vartheta_{vj} + N^{zz} \cos^2 \vartheta_{vj}). \end{aligned} \quad (33)$$

Then

$$\mathcal{L}(\vartheta(y)) = \alpha \left(\frac{d\vartheta}{dy} \right)^2 + \alpha' \left(\frac{d\vartheta}{dy} \right) + \frac{K}{a^3} \sin^2 \vartheta + \frac{(g\beta)^2}{a^6} V [N^{xx} \sin^2 \vartheta + N^{zz} \cos^2 \vartheta] \quad (34)$$

on the lowest level of approximation with respect to the angular distribution of magnetization.

6. Existence of domain structure at zero absolute temperature

As the first consequence of formula (34), for the mean value of the Hamiltonian we show that the domain structure assumed in Section 3 does exist. To this purpose we assume (a) that our domains in the form of stripes with the widths Δ can be treated as ellipsoids magnetized along the $\pm z$ axis, (b) that the regions of domains walls can be neglected,

(c) that the interaction between domains can be neglected. In this case, inside the domains we have $\cos^2 \vartheta = 1$, $\sin^2 \vartheta = 0$, and we can assume classical demagnetizing factor [13] as

$$N^{zz} = \frac{2\pi}{V} \frac{\Delta}{L_z} \frac{L_x}{L_z} \int_0^{\pi/2} \frac{\sin^2 \varphi d\varphi}{\sqrt{1-e^2 \sin^2 \varphi}}, \quad e = 1 - \left(\frac{\Delta}{L_z}\right)^2. \quad (35)$$

Here, when the width of domains Δ is comparable with the dimension L_z of the film along the z axis, we have $e \approx 0$ and

$$N^{zz} \approx \frac{\pi^2}{2V} \frac{\Delta L_x}{L_z^2}. \quad (36)$$

If there are s domains in the film, i.e. $L_y = s\Delta$, the average value of the Hamiltonian (34) is

$$\langle \mathcal{H} \rangle = \langle \mathcal{H}_0 \rangle + \frac{N}{4} \left\{ \frac{a^3}{\Delta} \sigma + \frac{(g\beta)^2}{a^3} \frac{\pi^2}{2} \frac{\Delta L_x}{L_z^2} \right\}, \quad (37)$$

where

$$\sigma = \frac{1}{S} \int_0^{L_y} \left[\alpha \left(\frac{d\vartheta}{dy} \right)^2 + \alpha' \left(\frac{d\vartheta}{dy} \right) \right] dy \quad (38)$$

represents the energy of the wall per unit of the wall surface. Minimizing (37) with respect to Δ we get

$$\Delta = \frac{\sqrt{2}}{\pi} \frac{a^3}{g\beta} \frac{L_z}{L_x^{1/2}} \sqrt{\sigma}. \quad (39)$$

From formula (39) it is possible to obtain the critical film thickness L_x^{crit} above which the domains exist. Namely, for films with $L_x = L_y$ from the condition $\Delta = L_z$ we obtain

$$L_x^{\text{crit}} = \frac{2}{\pi^2} \left(\frac{a^3}{g\beta} \right)^2 \sigma. \quad (40)$$

It is worth-while to notice that this result is in complete agreement with the result of the phenomenological theory [14], as well as with that of the theory based on the Heisenberg model [15]. In formulae (39) and (40) σ denotes the energy of the wall with zero width. It is not a real case, of course. Therefore, in the next Section we consider the structure of domain walls, and the wall energy σ obtained for this structure is substituted into (39) and (40).

7. The Bloch and Néel walls

We consider now the structure of the Bloch walls. For this purpose we assume that the Bloch walls with the width δ_B can be approximated by infinite cylinders magnetized along the x axis. We neglect the interaction between walls as well as between walls and domains. In this case we have [13]

$$N^{zz} = 0, \quad N^{xx} = 4\pi \frac{1}{V} \frac{\delta_B}{\delta_B + L_x}. \quad (41)$$

Then, the average value of Hamiltonian (34) is

$$\langle \mathcal{H} \rangle = \langle \mathcal{H}_0 \rangle + \frac{V}{\Delta} \int_{-A/2}^{+A/2} dy \left\{ A \left(\frac{d\vartheta}{dy} \right)^2 + R \sin^2 \vartheta \right\}, \quad (42)$$

where

$$A = \frac{1}{4} \alpha \quad (43)$$

$$R = \frac{1}{4} \left[\frac{K}{a^3} + \left(\frac{g\beta}{a^3} \right)^2 \frac{4\pi\delta_B}{\delta_B + L_x} \right]. \quad (44)$$

The minimization of formula (42) leads to the equation

$$2A \frac{d^2\vartheta}{dy^2} - R \sin 2\vartheta = 0. \quad (45)$$

The solution of this equation with the periodical boundary condition $\vartheta = \pi(n-1)$ for $y = (n-\frac{1}{2})\Delta$, ($n = 0, \pm 1, \pm 2, \dots$) can be written as

$$\cos \vartheta = \operatorname{sn} \left[\frac{2K(k)}{\Delta} y \right]. \quad (46)$$

Here sn denotes the elliptic sine function and $K(k)$ is the complete elliptic integral of the first kind with the modulus k connected to the domain width Δ by the relation

$$\kappa_0 \Delta = 2kK(k), \quad (47)$$

where

$$\kappa_0 = \sqrt{\frac{R}{A}}. \quad (48)$$

Taking into account that for real situations $\Delta\kappa_0 \gg 1$, it is a good approximation to substitute $k \simeq 1$.

Now, we can obtain the width of the Bloch walls

$$\delta_B = \frac{\pi}{\left(\frac{d\vartheta}{dy} \right)_{\vartheta=\pi/2}} = \frac{\pi}{\kappa_0} (1 - e^{-\Delta\kappa_0})^{1/2} \simeq \pi \sqrt{\frac{A}{R}}, \quad (49)$$

and the wall energy per unit of the wall surface

$$\sigma_B = \Delta \left\{ R \left(1 - \frac{1}{k^2} \right) + \frac{1}{\Delta} \frac{4}{k} E(k) \sqrt{AR} \right\} \simeq 4 \sqrt{AR}, \quad (50)$$

where $E(k)$ is the complete elliptic integral of the second kind.

Taking into account formula (44) we obtain for the Bloch wall width the equation

$$\frac{\delta_B}{a} = \frac{\pi}{a} \left(\frac{A}{K_u} \right)^{1/2} \left\{ 1 + \frac{4\pi M_s^2}{K/4a^3} \frac{\delta_B}{\delta_B + L_x} \right\}^{-1/2}, \quad (51)$$

where $M_s = g\beta S a^{-3}$ and

$$K_u = K(4a^3)^{-6}. \quad (52)$$

To consider the Néel walls we assume that the Néel walls with the width δ_N can be approximated by infinite cylinders magnetized along the x axis and we neglect the interaction between walls as well as between walls and domains. In this case we have [13]

$$N^{zz} = 0, \quad N^{yy} = 4\pi \frac{1}{V} \frac{L_y}{L_y + \delta_N}. \quad (53)$$

If we make the formal substitution $x \rightleftharpoons y$ in all formulae for the Bloch walls we get for the Néel walls

$$\frac{\delta_N}{a} = \frac{\pi}{a} \left(\frac{A}{K_u} \right)^{1/2} \left\{ 1 + \frac{4\pi M_s^2}{K_u} \frac{L_y}{L_y + \delta_N} \right\}^{-1/2}. \quad (54)$$

We can see from formulae (51) and (54) that the results of the band theory are in complete agreement with the results of the phenomenological theory [16] as well as with the results of that based on the Heisenberg model [17]. From the comparison of the last result with our result in the present paper we can see that the pseudodipolar anisotropic constant C [17] plays the role of the microscopic anisotropy parameter K and the role of the Heisenberg exchange parameter I [17] is taken by

$$A = \frac{1}{N} B a^{-1} \sum_{\tau hm} \langle n_{\tau hm} \rangle \cos h \gamma a \quad (55)$$

of this paper. Taking into consideration the condition of the minimum of the average value of the Hamiltonian for a given film thickness we can obtain the critical thickness below which the Néel walls are favourable and above which the Bloch walls occur.

However, in the framework of the band model, the influence of new additional factors on domain wall properties can also be investigated. One of these factors is connected with the inhomogeneity of spontaneous magnetization across a film, which appears in the band model even at $T = 0\text{K}$ [7]. Taking into account the spatial distribution of magnetization in the particular form given in [7]

$$\langle S_v^z \rangle = 1 + \frac{1}{2\pi n} - \frac{1}{2\pi} \frac{\delta_{1v} + \delta_{nv}}{2}, \quad (56)$$

we obtain

$$\frac{1}{n} \sum_v \langle S_v^z \rangle^2 = 1 + \frac{1}{8\pi^2 n} \left(1 - \frac{2}{n}\right) \quad \text{and} \quad \frac{1}{n} \sum_v \langle S_v^z \rangle = 1. \quad (57)$$

Then, we can see from formula (22) that the functional (42) retains its form, but instead of the coefficient R the changed coefficient R must be introduced for the Bloch walls:

$$R = \frac{1}{4} \left\{ \frac{K}{a^3} \left[1 + \frac{a}{8\pi^2 L_x} \left(1 - \frac{2a}{L_x}\right) \right] + \left(\frac{g\beta}{a^3} \right)^2 \frac{4\pi\delta_B}{\delta_B + L_x} \right\}. \quad (58)$$

In consequence, the effective anisotropy constant Ku determined by (52) must be corrected by the factor in the square brackets of (58); this factor is a function of the film thickness. Thus, the slope of the Bloch wall width vs film thickness curve is greater than in the case when the spontaneous magnetization is considered to be homogeneous. This fact is in qualitative agreement with some experiments concerning the domain wall width [18]. However, the values of the Bloch wall widths measured by means of Lorentz microscopy are still too large in comparison with theoretical ones (this is caused, of course, by the inelastic scattering of electrons [18]). The decrease of the Bloch wall width calculated here depends on the surface conditions and is more important when the surfaces are not magnetized. In particular, the appearance of magnetically dead layers [19] enlarges the domain wall width. Effects described above appear, of course, also for the Néel walls.

Another effect which can be discussed only for the band model approach is the dependence of the stiffness parameter A on the film thickness and surface the conditions [20]. This parameter decreases for very thin films and so leads to a decrease of the domain wall width if the film thickness is below some critical value [20]. Fortunately, the Bloch walls are usually observed above this critical value, where the stiffness parameter is practically constant. For special surface conditions [20], however, we should expect a drastic jump of the domain wall width in the region of the critical value of the film thickness.

Moreover, it is worth-while to notice that there is one more effect which can be treated only in the framework of the band model, namely, the distribution of the quantization axes in domain walls for different states of electrons. This effect was investigated separately [5] and will not be treated here.

8. Conclusions

For simplicity, three basic approximations are used for the formulation of the problem in question:

1. Instead of the real Hamiltonian responsible for anisotropy effects in the band model of ferromagnetism we use some kind of an effective anisotropy Hamiltonian, the form of which is based on the argument of utility only.

2. We take an approximate form of the diagonalization procedure assuming that the diagonal form of the Hamiltonian is assured by the Fourier transformation in the film plane (both along the domains as well as across them) and a special transformation

in the direction perpendicular to the film plane. From the calculation for the Heisenberg model we know that the Fourier transformation in the direction across the domains constitutes only the first approximation in the sense of the perturbation theory to the complete diagonalization. In the light of the more rigorous recent considerations given in the paper [21] we can see that the mentioned approximation is fully justified.

3. The long range magnetic dipolar interactions are treated by means of demagnetizing factors which is a good approximation only for a one ellipsoidal domain. From phenomenological theories we know that such kind of approximation is only qualitatively justified in our case and that realistic solutions are much more complicated than those found in this paper.

Apart from these simplifications, without which the problem in question would be very complicated, we can say that the formulation of the band model in a form permitting the description of the domain structure in thin films at zero absolute temperature is really obtained in this paper and that our qualitative results are in complete agreement with those of the classical approaches. In particular, parameters characterizing the domain structure (the domain width Δ , the wall width δ , the wall energy σ , the critical thickness above which the domain structure can exist) were calculated.

Moreover, our theory allows us to obtain the stiffness parameter A and to find the relation between the Heisenberg exchange integral I and the hopping parameter B of the band theory. It is very interesting that the stiffness parameter A depends on the film thickness as well as on the surface conditions. We were able also to obtain the film thickness dependence of the effective anisotropy constant. Finally, it is worth-while to notice that our approach allows us also to consider other effects which can be explained only in the framework of the band model approach. We can mention here the distribution of the quantization axes in domain walls for different states of electrons, which was investigated separately, as well as the dependence of the demagnetizing term on the electronic distribution inside the elementary cell, the role of which will be important only when the exact quantum mechanical approach to the demagnetizing field will be successfully applied.

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