BAND MODEL APPROACH TO THE THEORY OF DOMAIN STRUCTURE*

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Within the framework of the band model of ferromagnetism a uniform and consistent approach to the problem of domain structure is presented. The Hamiltonian consisting of the Hubbard term and the pseudodipolar term is taken as a starting point. The Green function formalism is introduced and the angular distribution of magnetization directions in domain walls, wall widths as well as domain widths are derived. Influence of external magnetic fields on domain structure is also investigated. The approach has rather a fundamental meaning but it allows one to reach certain results which cannot be obtained in other models.

1. Introduction

Many experimental and theoretical papers dealt with the problem of domain structure in ferromagnets but only recently an attempt has been made to solve the problem within the framework of the band model of ferromagnetism [1–4]. In this approach the existence of a definite structure is assumed and the angular distribution of magnetization directions in the domain walls as well as the basic domain and wall parameters are calculated. Up to now the most unsatisfactory feature of this theory is the phenomenological description of magnetic anisotropy. A more accurate approach requires this anisotropy to be introduced in a microscopical and consistent form. The best solution of the problem would be to take into account the spin-orbit interaction in the Hamiltonian explicitly. Calculations of anisotropy, with the spin-orbit interaction as a starting point, were performed indeed some years ago and the anisotropy constants for Ni and Fe were obtained [5–11]. Unfortunately, the method is complicated to such an extend that it seems to be ineffective for such problems as the problem of domain structure. Therefore, a simpler approach, based on the pseudodipolar Hamiltonian, is probably much more appropriate for this purpose. As a matter of fact, it represents a rather rough way of treating the anisotropy effects, but it allows one to obtain, in an easy way, the expressions for anisotropy constants

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as functions of basic energy band parameters [12]. For our purpose it is, as we will see, important that this approach is fully useful for the theory of domain structure.

The aim of the present paper is to investigate domain structure problems within the framework of the band model of ferromagnetism, by using the Hubbard Hamiltonian complemented by the pseudodipolar term. The approach may be treated as completely consistent and uniform, because the magnetocrystalline anisotropy is introduced here by a term which can be presented in a form consistent with the Hubbard Hamiltonian. The difficulty associated with demagnetizing effects which are not taken into account in the Hamiltonian explicitly is avoided by assuming a stray-field-free domain configuration of Landau-Lifshitz type. We treat internal domains and surface closure domains as independent and additive, so we perform all calculations separately for each parts of the domain structure. For internal domains, the angular distribution of magnetization directions in the Bloch walls as well as basic wall parameters will be found. Next, with the surface flux closure structure introduced, the domain width will be calculated. The influence of the external magnetic field on the ferromagnet with domains will be also discussed. In order to simplify calculations we will take under consideration a crystal of simple hexagonal structure with the z-axis along the hexagonal axis.

The problem in question was already discussed by us in the form of a short digest [13]; this paper presents the theory in a more detailed and extensive way.

2. *The Hamiltonian*

As a starting point of the presented theory, the Hamiltonian consisting of the isotropic Hubbard term and the pseudodipolar term responsible for anisotropy effects is taken as

$$\mathscr{H} = \mathscr{H}_I + \mathscr{H}_A, \tag{1}$$

where

$$\mathscr{H}_I = \sum_{\langle ij\rangle\sigma} T_{ij} b_{i\sigma}^{+} b_{j\sigma} + I \sum_i b_{i\uparrow}^{+} b_{i\uparrow} b_{i\downarrow}^{+} b_{i\downarrow} \tag{2}$$

and

$$\mathscr{H}_A = \sum_{\langle ij\rangle} D_{ij} [\boldsymbol{S}_i \boldsymbol{S}_j - 3 r_{ij}^{-2} (\boldsymbol{S}_i \boldsymbol{r}_{ij}) (\boldsymbol{S}_j \boldsymbol{r}_{ij})]. \tag{3}$$

In the above expressions, $b_{i\sigma}^{+}$, $b_{i\sigma}$ denote creation and annihilation operators of electrons with the spin $\sigma = \uparrow$ or $\downarrow$ in the Wannier representation at the lattice point $\boldsymbol{i}$. T_{ij} is the hopping integral from the lattice point $\boldsymbol{i}$ to its nearest neighbour $\boldsymbol{j}$ and I represents the intraatomic Coulomb interaction between electrons. The pseudodipolar constant D_{ij} equals D if the sites $\boldsymbol{i}$ and $\boldsymbol{j}$ are the nearest neighbours and 0 otherwise; $\boldsymbol{r}_{ij}$ is the radius vector and $\boldsymbol{S}_i$ is the spin operator, the components of which in the second quantization representation are:

$$S_i^x = \tfrac{1}{2} \sum_\sigma b_{i\sigma}^{+} b_{i-\sigma}, \qquad S_i^y = -\frac{i}{2} \sum_\sigma \hat{\sigma} b_{i\sigma}^{+} b_{i-\sigma}, \qquad S_i^z = \tfrac{1}{2} \sum_\sigma \hat{\sigma} b_{i\sigma}^{+} b_{i\sigma},$$

where $\hat{\sigma} = +1$ for $\sigma = \uparrow$ or -1 for $\sigma = \downarrow$.

Then, the pseudodipolar Hamiltonian $\mathscr{H}_A$ in the second quantization representation takes the form

$$\mathscr{H}_A = \sum_{i \neq j} \{A_{ij}(b_{i\uparrow}^+ b_{i\uparrow} b_{j\downarrow}^+ b_{j\downarrow} + b_{i\uparrow}^+ b_{i\downarrow} b_{j\downarrow}^+ b_{j\uparrow} - \tfrac{1}{2} b_{i\uparrow}^+ b_{i\uparrow} b_{j\uparrow}^+ b_{j\uparrow} - \tfrac{1}{2} b_{i\downarrow}^+ b_{i\downarrow} b_{j\downarrow}^+ b_{j\downarrow})$$

$$+ B_{ij} b_{i\uparrow}^+ b_{i\downarrow} b_{j\uparrow}^+ b_{j\downarrow} + C_{ij} b_{i\uparrow}^+ b_{i\downarrow} (b_{j\uparrow}^+ b_{j\uparrow} - b_{j\downarrow}^+ b_{j\downarrow}) + \text{h.c.}\}, \tag{4}$$

where

$$A_{ij} = -\tfrac{1}{4} D_{ij} \left[1 - 3\left(\frac{r_{ij}^z}{r_{ij}}\right)^2\right], \tag{5}$$

$$B_{ij} = -\tfrac{3}{8} D_{ij} \frac{(r_{ij}^x - i r_{ij}^y)^2}{r_{ij}^2}, \tag{6}$$

$$C_{ij} = -\tfrac{3}{4} D_{ij} \frac{r_{ij}^z (r_{ij}^x - i r_{ij}^y)}{r_{ij}^2}. \tag{7}$$

3. Angular distribution of magnetization directions in the internal domain walls

The internal part of domain structure is assumed to consist of plates of width Δ, magnetized antiparallelly and separated by 180° Bloch walls. To describe this domain structure, Hamiltonian (1) is expressed in terms of operators c_i defined as follows [2]:

$$b_{i\sigma} = \cos\frac{\vartheta_i}{2} c_{i\sigma} - \hat{\sigma} \sin\frac{\vartheta_i}{2} c_{i-\sigma}. \tag{8}$$

This transformation represents a rotation of the spin operator $\boldsymbol{S}_i$ by an angle ϑ_i about the y-axis, perpendicular to the domain walls. The angle ϑ is measured with recpect to the easy axis and depends only on y.

Hamiltonian (1) is approximately diagonalized by means of the three-dimensional Fourier transformation

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\tau h} e^{-i(h_x i_x - h_z i_z)} e^{-i\tau i_y} \beta_{\tau h \sigma} \tag{9}$$

The fact that the rotation of the magnetization vector inside the Bloch walls is gradual and rather slow allows us to treat the angle ϑ as a continuous function of y and introduce the following approximation: $\vartheta_{i+\Delta i} \simeq \vartheta_i + \Delta i \nabla \vartheta_i$. This fact allows us also to assume that transformation (9) diagonalizes the Hamiltonian with respect to the indices τ, connected with the direction perpendicular to domain walls.

The mean energy of the system is calculated by using the Green function formalism in a similar way as in paper [2]. Green functions of the type $G_{\tau h}^{\sigma\sigma'} = \langle\langle \beta_{\tau h\sigma}; \beta_{\tau h\sigma'}^{+} \rangle\rangle_E$ are introduced and the Hartree-Fock procedure of decoupling e. g.

$$\sum_{\substack{\tau' h' \\ tm}} \langle\langle \beta_{\tau'+th'+m-\sigma}^{+} \beta_{\tau' h'-\sigma} \beta_{\tau+th+m\sigma}; \beta_{\tau h\sigma'}^{+} \rangle\rangle_E \simeq \sum_{\tau' h'} \langle \beta_{\tau' h'-\sigma}^{+} \beta_{\tau' h'-\sigma} \rangle \langle\langle \beta_{\tau h\sigma}; \beta_{\tau h\sigma'}^{+} \rangle\rangle_E \tag{10}$$

leads to the following equations of motion

$$(E - \mathscr{F}_{\tau h} - In_{-\sigma} - E_{\tau h\sigma}^{A}) G_{\tau h}^{\sigma\sigma} - \Gamma_{\tau h\sigma} G_{\tau h}^{-\sigma\sigma} = \frac{1}{2\pi} \tag{11}$$

$$(E - \mathscr{F}_{\tau h} - In_{\sigma} - E_{\tau h-\sigma}^{A}) G_{\tau h}^{-\sigma\sigma} - \Gamma_{\tau h-\sigma} G_{\tau h}^{\sigma\sigma} = 0, \tag{12}$$

where

$$\mathscr{F}_{\tau h} = \varepsilon_{\tau h} + \tfrac{1}{8} \varepsilon_{\tau h}^{(2)} \overline{\left(\frac{d\vartheta}{dy}\right)^2}, \tag{13}$$

$$\overline{\left(\frac{d\vartheta}{dy}\right)^2} = \frac{1}{2\Delta} \int_{-\Delta}^{\Delta} dy \left(\frac{d\vartheta}{dy}\right)^2, \qquad \varepsilon_{\tau h}^{(i)} = \frac{\partial^{(i)} \varepsilon_{\tau h}}{\partial \tau^{(i)}},$$

$\varepsilon_{\tau h}$ is here the Bloch energy,

$$n_{\sigma} = \frac{1}{N} \sum_{\tau h} n_{\tau h\sigma} = \frac{1}{N} \sum_{\tau h} \langle \beta_{\tau h\sigma}^{+} \beta_{\tau h\sigma} \rangle \tag{14}$$

is a number of electrons per atom,

$$E_{\tau h\sigma}^{A} = \frac{\hat{\sigma}\mu}{2} \Bigg\{ -2A_{00} + 3A_{00} \overline{\sin^2 \vartheta} + \tfrac{1}{2} A_{00}^{(2)} \overline{\left(\frac{d\vartheta}{dy}\right)^2}$$

$$- \frac{1}{N\mu} \sum_{tm\sigma_1} \hat{\sigma}_1 \left[-2A_{tm} + (3A_{tm} + B_{tm} + B_{tm}^{*}) \overline{\sin^2 \vartheta} + \tfrac{1}{2} (A_{tm}^{(2)} + B_{tm}^{(2)} + B_{tm}^{(2)*}) \overline{\left(\frac{d\vartheta}{dy}\right)^2} \right] n_{\tau+th+m\sigma_1}$$

$$- \frac{\hat{\sigma}}{2N\mu} \sum_{tm} (-A_{tm}^{(2)} + B_{tm}^{(2)} + B_{tm}^{(2)*}) \overline{\left(\frac{d\vartheta}{dy}\right)^2} n_{\tau+th+m-\sigma}$$

$$- \frac{i}{N\mu} \sum_{tm} (B_{tm}^{(1)} - B_{tm}^{(1)*}) \overline{\sin\vartheta \frac{d\vartheta}{dy}} n_{\tau+th+m-\sigma} \Bigg\}, \tag{15}$$

$$\mu = \frac{1}{N} \sum_{\tau h\sigma} \hat{\sigma} n_{\tau h\sigma} \tag{16}$$

is the spontaneous magnetization,

$$\Gamma_{\tau h\sigma} = -\frac{i\hat{\sigma}}{2}\frac{\pi}{\Delta}\varepsilon_{\tau h}^{(1)} + \frac{i\hat{\sigma}}{4N}\sum_{tm\sigma_1}\left[(A_{tm}^{(1)} - B_{tm}^{(1)} - B_{tm}^{(1)*})\overline{\frac{d\vartheta}{dy}}\right.$$

$$\left. + \frac{\hat{\sigma}}{2}(C_{tm}^{(1)} - C_{tm}^{(1)*})\overline{\sin\vartheta\frac{d\vartheta}{dy}}\right] n_{\tau+th+m\sigma_1} - \frac{1}{4N}\sum_{tm\sigma_1}\hat{\sigma}_1\left[(C_{tm} + C_{tm}^*)(2\overline{\cos^2}\vartheta - 1)\right.$$

$$\left. - \tfrac{1}{2}(C_{tm}^{(2)} + C_{tm}^{(2)*})\overline{\left(\frac{d\vartheta}{dy}\right)^2}\right] n_{\tau+th+m\sigma_1}. \tag{17}$$

A_{tm}, B_{tm}, C_{tm} in the above expressions are the Fourier transforms of the coefficients A_{ij}, B_{ij}, C_{ij}, respectively.

Then, the self-consistent set of equations for the mean energy E of the system, the number n of electrons per atom and for the spontaneous magnetization μ is the following

$$E = \sum_{\tau hs} E_{\tau hs} f(E_{\tau hs}) - \langle \mathscr{H}_{\text{int}} \rangle, \tag{18}$$

$$n = \frac{1}{N}\sum_{\tau hs} f(E_{\tau hs}), \tag{19}$$

$$\mu = \frac{1}{N}\sum_{\tau hs}\frac{g_{\tau h}}{(g_{\tau h}^2 + 4\Gamma_{\tau h\uparrow}\Gamma_{\tau h\downarrow})^{1/2}}\hat{s} f(E_{\tau hs}), \tag{20}$$

where

$$E_{\tau hs} = \mathscr{F}_{\tau h} + \tfrac{1}{2} In - \frac{1}{8N}\sum_{tm\sigma_1}\left[(-A_{tm}^{(2)} + B_{tm}^{(2)} + B_{tm}^{(2)*})\overline{\left(\frac{d\vartheta}{dy}\right)^2}\right.$$

$$\left. - 2i\hat{\sigma}_1(B_{tm}^{(1)} - B_{tm}^{(1)*})\overline{\sin\vartheta\frac{d\vartheta}{dy}}\right] n_{\tau+th+m\sigma_1} - \frac{\hat{s}}{2}(g_{\tau h}^2 + 4\Gamma_{\tau h\uparrow}\Gamma_{\tau h\downarrow})^{1/2}, \tag{21}$$

$$g_{\tau h} = I\mu - (E_{\tau h\uparrow}^A - E_{\tau h\downarrow}^A) \tag{22}$$

and $\hat{s} = \pm 1$. The function $f(E_{\tau hs})$ denotes here the Fermi–Dirac distribution function and

$$\mathscr{H}_{\text{int}} = \frac{I}{N}\sum_{\substack{\tau h\tau' h' \\ tm}}\beta_{\tau+th+m\uparrow}^{+}\beta_{\tau'-th'-m\downarrow}^{+}\beta_{\tau' h'\downarrow}\beta_{\tau h\uparrow} + \mathscr{H}_A.$$

The set of equations (18)–(20) is solved by an iterative method. As a zeroth approximation we take $\mu = \mu_0$, $n_{\tau hs} = n_{\tau h\sigma}^0$ where index zero refers to the homogeneously magnetized state. Besides, it is assumed that: (*i*) the pseudodipolar coupling constant D is small both in comparison to the intraatomic Coulomb interaction I and to the bandwidth, (*ii*) the

distribution function of occupation numbers for the Hartree-Fock one electron states is the same as for homogeneously magnetized state, i. e.

$$f(E_{\tau hs}) \simeq f(E^0_{\tau h\sigma}) = n^0_{\tau h\sigma}.$$

Hence, the mean energy of the internal part of the domain structure (in the second iterational step) is equal to

$$E_1 = E_{01} + \frac{\Omega}{2\Delta}\int_{-\Delta}^{\Delta}\left[A\left(\frac{d\vartheta}{dy}\right)^2 - K\cos^2\vartheta\right]dy - \frac{\pi^2}{4I\mu_0\Delta^2}\sum_{\tau h\sigma}\hat{\sigma}\left(\frac{\partial\varepsilon_{\tau h}}{\partial\tau}\right)^2 n^0_{\tau h\sigma}, \tag{23}$$

where E_{01} is the energy of the system for the homogeneously magnetized state, Ω is the volume of the internal region and

$$A = \frac{1}{8\Omega}\sum_{\tau h\sigma}\frac{\partial^2\varepsilon_{\tau h}}{\partial\tau^2}n^0_{\tau h\sigma}. \tag{24}$$

In formula (23), K has the meaning of the uniaxial anisotropy constant. For the simple hexagonal structure the following expression is found

$$K = \frac{3\mu_0^2 N}{\Omega}[3D_1(b_{100}-1) - 2D_2(b_{001}-1)]. \tag{25}$$

D_1, D_2 describe here pseudodipolar couplings between nearest neighbours in the same and in the adjacent hexagonal planes, respectively, whereas functions b_h are defined as follows

$$b_h = \frac{1}{N^2\mu_0^2}\sum_{km\sigma\sigma'}\hat{\sigma}\hat{\sigma}' e^{i(m-k)r_h} n^0_{k\sigma} n^0_{m\sigma'}. \tag{26}$$

According to Eqs. (25) and (26), the uniaxial anisotropy constant depends essentially on band parameters such as the Fermi level position in the band and occupation numbers for one-electron Hartree-Fock states [12].

Energy E_1 (Eq. (23)) is a functional of the angular distribution of magnetization directions $\vartheta(y)$. Minimization with respect to ϑ leads to the relation

$$\cos\vartheta = -\mathrm{sn}\left[\frac{2\mathscr{K}}{\Delta}y + \mathscr{K}\right], \tag{27}$$

where sn denotes the Jacobi elliptical function and $\mathscr{K}$ is the complete elliptical integral of the first kind.

For the wall width and the wall energy we obtain, respectively

$$\delta = \pi\sqrt{\frac{A}{K}}, \tag{28}$$

$$\sigma = 4\sqrt{AK} - \frac{\pi^2}{4I\mu_0\Delta\Omega}\sum_{\tau h\sigma}\hat{\sigma}\left(\frac{\partial\varepsilon_{\tau h}}{\partial\tau}\right)^2 n^0_{\tau h\sigma}. \tag{29}$$

As we see, working within the framework of the band model of ferromagnetism, we have found the distribution of magnetization directions and the domain wall width identical as in the phenomenological [14] and Heisenberg model [15] approaches. As far as the Bloch wall energy is concerned, we have obtained a lower value than in other models (analogically as in paper [2]). The difference is associated with the decrease in magnetization in the walls in comparison to its value in the homogeneously magnetized state. Namely, the following expression for magnetization has been derived

$$\mu \simeq \mu_0 - \frac{\pi^2}{2NI^2\mu_0^2\Delta^2} \sum_{\tau h\sigma} \hat{\sigma} \left(\frac{\partial \varepsilon_{\tau h}}{\partial \tau}\right)^2 n^0_{\tau h\sigma}. \tag{30}$$

The physical cause of the decrease in magnetization (and consequently of energy) is the deviation of quantization axes of electrons from the direction of macroscopical magnetization [1]. Here it should be stressed that only the band model approach allows one to introduce the dependence of quantization axes of electrons on their quantum state; in other models this is not possible. (In the Heisenberg model, a decrease in magnetization in domain walls was also obtained [16, 17], but it was attributed to by other effects).

It is worth-while to make some remarks concerning the so-called stiffness parameter. The quantity A (Eq. (24)) influences the angular distribution of the magnetization vector and the domain wall width, so it may be interpreted as the wall stiffness parameter. We can see however that this parameter (defined here on the base of domain structure theory) is different from that introduced in the spin-wave theory [18]. Namely, the spin wave stiffness parametr is defined as a measure of the increase in the crystal energy associated with the transversal inhomogenity of magnetization [18]. This definition refers, of course, to a case with anisotropy not taken into account. If we exclude anisotropy from our calculation, the rotation of the magnetization vector in the walls is linear, and from Eq. (23)

$$\Delta E = E_1 - E_{01} = \left(\frac{\pi}{\Delta}\right)^2 \frac{1}{8\Omega} \sum_{\tau h\sigma} \left[\frac{\partial^2 \varepsilon_{\tau h}}{\partial \tau^2} - \frac{2}{I\mu_0} \hat{\sigma} \left(\frac{\partial \varepsilon_{\tau h}}{\partial \tau}\right)^2\right] n^0_{\tau h\sigma}. \tag{31}$$

In this case, we obtain the spin wave stiffness parameter analogicaly as in paper [18].

The physical cause of both parameters (the spin wave stiffness parameter and the wall stiffness parameter) is the kinetic energy of itinerant electrons. The difference between them is associated with the decrease in the magnetization value in the Bloch walls.

4. Estimation of the domain width

To calculate the domain width Δ we minimize the total energy of the system (the stray-field-free domain configuration of the Landau-Lifshitz type) with respect to Δ. We assume the total energy to be a sum of the internal and the surface region energies. The energy of the internal part has been calculated in the previous section. To describe

the surface domain structure, Hamiltonian (1) is expressed by means of other operators $c_{i\sigma}$, which now should be defined as follows

$$b_{i\sigma} = \left(\cos\frac{\vartheta_i}{2} - \frac{i\hat{\sigma}}{\sqrt{2}}\sin\frac{\vartheta_i}{2}\right)c_{i\sigma} - \frac{\hat{\sigma}}{\sqrt{2}}\sin\frac{\vartheta_i}{2}\,c_{i-\sigma}. \tag{32}$$

The above transformation describes the rotation of the spin operator $\boldsymbol{S}_i$ about the axis perpendicular to the closure domain walls by an angle ϑ. The angle ϑ depends in this case on two variables: y and z.

The energy E_2 of the surface region is calculated in the same way as for the internal part of the domain structure. Minimization of E_2 with respect to $\vartheta(y, z)$ gives the following distribution of magnetization directions (we assume that I is large as compared to the bandwidth) [3]

$$\cos\vartheta = \frac{k^2 - \operatorname{sn} t}{1 - k^2 \operatorname{sn} t}, \qquad \sin\vartheta = (1-k^4)^{1/2}\frac{\operatorname{cn} t}{1 - k^2 \operatorname{sn} t}, \tag{33}$$

where

$$t = \frac{2\mathcal{K}}{\Delta}(y+z)$$

and k is the modulus of the elliptical functions.

A domain structure which corresponds to distribution function (33) is slightly different than that taken as a starting point (Landau-Lifshitz structure) since the magnetic flux is not entirely contained within the crystal. Therefore, the Landau-Lifshitz structure should be treated only as a zeroth approximation of the iteration [3]. Similar results were obtained in the Heisenberg model [15].

The energy of closure domains minimized with respect to the distribution function $\vartheta(y, z)$ is equal to

$$E_2^{\min} = E_{02} + \tfrac{3}{4} K\varepsilon L_x L_y \Delta, \tag{34}$$

where E_{02} is the part of surface region energy independent of Δ,

$$\varepsilon = \frac{4}{\Delta^2}\int_0^{\Delta/2} dy \int_0^{\Delta/2} dz \sin^2\vartheta, \tag{35}$$

and L_i is the crystal dimension in the direction of the i-axis ($i = x, y, z$).

Now, it is possible to calculate the domain width. Minimizing the total energy of Landau-Lifshitz structure with respect to Δ(ε is treated as a constant) we obtain the well-known relation

$$\Delta = CL_z^{1/2}, \tag{36}$$

where

$$C = \frac{4}{(3\varepsilon)^{1/2}}\left(\frac{A}{K}\right)^{1/4}.$$

5. *Influence of the external magnetic field*

Here, we will consider the influence of external magnetic fields on the internal part of the domain structure only, because calculations which take into account the surface region, even in the simplest form, become very complicated.

Now, the anisotropic Hamiltonian (1) should be complemented by a term $\mathscr{H}_F$ which describes the interaction of the spin system with an external magnetic field of strength H. Therefore

$$\mathscr{H} = \mathscr{H}_I + \mathscr{H}_A + \mathscr{H}_F, \tag{37}$$

where $\mathscr{H}_I$ and $\mathscr{H}_A$ are given by Eqs. (2) and (4) whereas $\mathscr{H}_F$, in the second quantization representation, takes a form

$$\mathscr{H}_F = -\tfrac{1}{2}\, g\mu_B \sum_i (H^x b_{i\sigma}^+ b_{i-\sigma} - i\hat{\sigma} H^y b_{i\sigma}^+ b_{i-\sigma} + \hat{\sigma} H^z b_{i\sigma}^+ b_{i\sigma}). \tag{38}$$

In the above expression, μ_B is the Bohr magneton and g represents the Lande splitting factor. To take into account the domain structure Hamiltonian (37) should be expressed by means of the operators $c_{i\sigma}$ defined by the transformation (8).

The investigation of the influence of an arbitrarily directed external magnetic field encounters essential mathematical difficulties so only three simple cases will be discussed here: (*i*) magnetic field directed parallelly to the easy axis, (*ii*) magnetic field perpendicular to the easy axis and parallel to the Bloch walls, (*iii*) magnetic field perpendicular both to the easy axis and the Bloch walls.

The mean energy of the system is calculated in each case analogically as in paper [4] but now Hamiltonian (37) is taken as a starting point.

The following results are obtained

Case (*i*)

$$E = E_{01} + \frac{\Omega}{N} K \frac{1}{L_y} \int_0^{L_y} dy \left\{ \frac{A}{K} \left(\frac{d\vartheta}{dy} \right)^2 - \cos^2 \vartheta - q \cos \vartheta \right\}$$

$$- \frac{\pi^2}{4NI\mu_0 \Delta^2} \sum_{\tau h \sigma} \hat{\sigma} \left(\frac{\partial \varepsilon_{\tau h}}{\partial \tau} \right)^2 n_{\tau h \sigma}^0, \tag{39}$$

where

$$q = \frac{\mu_0 g \mu_B H}{2K \dfrac{\Omega}{N}} \tag{40}$$

and A, K are given by Eqs. (24) and (25).

Minimization of energy E with respect to ϑ leads to the distribution of magnetization directions analogical as in the phenomenological [14] and Heisenberg [19] models. The same result was obtained in paper [4]. The distribution function shows that in the

presence of a magnetic field parallel to the easy axis the domain boundaries shift in such a way that the volume of domains magnetized antiparallelly to the field approaches zero whereas the wall width does not change essentially.

Case (*ii*)

$$E = E_{01} + \frac{\Omega}{N} K \frac{1}{L_y} \int_0^{L_y} dy \left\{ \frac{A}{K} \left(\frac{d\vartheta}{dy} \right)^2 - \cos^2 \vartheta - q \sin \vartheta \right\}$$

$$- \frac{\pi^2}{4NI\mu_0 \Delta^2} \sum_{\tau h \sigma} \hat{\sigma} \left(\frac{\partial \varepsilon_{\tau h}}{\partial \tau} \right)^2 n^0_{\tau h \sigma}. \tag{41}$$

The distribution function obtained by the minimization of Eq. (41) with respect to ϑ shows that in a transversal magnetic field directed parallelly to the Bloch walls the magnetization vector rotates into the field direction [4, 20].

Case (*iii*)

$$E = E_{01} + \frac{\Omega}{N} K \frac{1}{L_y} \int_0^{L_y} dy \left\{ \frac{A}{K} \left(\frac{d\vartheta}{dy} \right)^2 - \cos^2 \vartheta \sin^2 \varphi - q \cos \varphi \right\}$$

$$- \frac{\pi^2}{4NI\mu_0 \Delta^2} \sum_{\tau h \sigma} \hat{\sigma} \left(\frac{\partial \varepsilon_{\tau h}}{\partial \tau} \right)^2 n^0_{\tau h \sigma}. \tag{42}$$

The system energy is now dependent on angles $\vartheta = \vartheta(y)$ and $\varphi = \varphi(H)$ which describe the direction of the magnetization vector. Minimization of Eq. (42) with respect to $\vartheta(y)$ and $\varphi(H)$ (analogically as in papers [4, 21]) leads to the result that an increase in the field strength causes angle ϑ to become gradually a linear function of y and the domain structure to transform into a spiral structure.

6. *Conclusions*

Introducing magnetocrystalline anisotropy by means of the pseudodipolar Hamiltonian gives a uniform, microscopical approach to domain structure problem within the framework of the band model.

According to this method angular distribution of magnetization directions in Bloch walls, basic wall parameters as well as the domain width Δ have been calculated. The obtained results are in agreement with those of the phenomenological and Heisenberg models. Moreover, the method allows one to find the expression for the anisotropy constant.

Therefore, it is possible to state that the domain structure problem can be really solved within the framework of the band model of ferromagnetism and it constitutes another approach to the discussed problem apart from the phenomenological and Heisenberg models.

Compared to the phenomenological model, this approach is of a fundamental rather than of practical significance. But, it should be pointed out that the investigation of domain structure in the band model leads to certain results which can not be reached in other theories. Namely, only in the band theory it is possible to introduce a dependence of quantization axes of electrons on their quantum states. As a consequence, a lower value of magnetization is found for the state with domain structure as compared to the value for the homogeneously magnetized state. So, the wall energy is lower than in phenomenological and Heisenberg models.

A modification of energy bands in the presence of domain structure as well as the position dependence of the length of the magnetization vector and of the number of electrons per atom are examples of other (not discussed here) results which can be obtained within the framework of the band model in a simple and natural way.

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