

PSEUDODIPOLAR THEORY OF MAGNETOCRYSTALLINE ANISOTROPY IN THE BAND MODEL OF FERROMAGNETISM*

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The pseudodipolar theory of magnetocrystalline anisotropy is discussed within the framework of the itinerant electron model. The first anisotropy constant K_1 for crystals having cubic and hexagonal symmetries is derived. It is pointed out that K_1 depends on basic band parameters such as the energy gap and Fermi energy. Some conclusions concerning the temperature dependence of K_1 are drawn. The usefulness of the model for other problems is also discussed.

1. Introduction

The aim of this paper is to elaborate a simple model of magnetocrystalline anisotropy within the framework of the band theory of ferromagnetism.

The problem of anisotropy was a subject of many experimental and theoretical papers. The microscopic theories were mostly based on the Heisenberg model [1] and only a few papers treating the problem in the itinerant electron model were published [2-9].

From the microscopic point of view the spin-orbit interaction is considered to be responsible for magnetocrystalline anisotropy. If a term describing this interaction is introduced into the Hamiltonian and the perturbation theory is used, it is possible to obtain an anisotropy energy term in the second order for crystals of hexagonal symmetry and in the fourth order for cubic crystals. Such calculations, with some other simplifications, were performed for nickel and iron [2-4]. But the obtained values of anisotropy constants were not in good agreement with the experimental data. Therefore, in subsequent papers these simplifications were successively rejected and it was shown that the deformation of the Fermi surface induced by spin-orbit interaction essentially influenced the anisotropy energy [5]. Moreover, it was derived for nickel that the existence of degenerate states near the Fermi surface gives a large contribution to anisotropy [6-8]. Recently,

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progress in evaluating of the real band structures for transition metals allowed one to perform the anisotropy calculations more exactly.

It should be pointed out that the aim of the mentioned papers was to obtain the best possible agreement between theoretical and experimental results concerning the anisotropy constants and their temperature dependence for transition metals. Because many additional effects had to be taken into account, the calculations became so complicated that it seemed ineffective to use such an approach for problems in which the magnetocrystalline anisotropy plays an important role as it is e. g. in the domain structure theory. Due to this fact, in previous investigations of domain structure using the band model, uniaxial anisotropy was described in the Hamiltonian merely by a term of the molecular field type with a generalized coefficient treated as a parameter [10]. More accurate considerations of domain structure require a consistent and microscopic method for introduction of anisotropy.

We see therefore, there are two different aspects of the anisotropy problem. On the one hand, very exact calculations are performed to obtain the best agreement with experimental data and on the other hand, very simple models are necessary to describe anisotropy in various problems.

In this paper we will deal with the latter aspect of anisotropy, which seems to us a particularly interesting one. Namely, within the framework of the band theory of ferromagnetism, we will present a model of magnetocrystalline anisotropy based on a pseudodipolar Hamiltonian. It will be shown that the anisotropy constant depends on basic band parameters, such as the energy gap and the Fermi energy. The simplicity of the model allows one to use it in various problems in which the anisotropy plays an important role. It should be effective in the domain structure theory as well as in investigations of the influence of anisotropy on spin wave energies.

2. The Hamiltonian

We assume that the Hamiltonian consists of two parts: H_I —describing isotropic interactions and H_A —responsible for anisotropy effects. So

$$H = H_I + H_A. \quad (1)$$

We take H_I in a form of the one-band Hubbard Hamiltonian

$$H_I = \sum_{ij\sigma} T_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + I \sum_i c_{i\uparrow}^{\dagger} c_i c_{i\downarrow}^{\dagger} c_i, \quad (2)$$

where $c_{i\sigma}^{\dagger}(c_{i\sigma})$ are creation (annihilation) operators of an electron with the spin $\sigma = \uparrow$ or \downarrow in the Wannier representation at the lattice point i . T_{ij} denote hopping integrals from the lattice point i to its nearest neighbour j and I represents the intra-atomic Coulomb interaction between electrons.

We choose H_A in a form of the pseudodipolar Hamiltonian

$$H_A = \frac{1}{2} \sum_{i \neq j} P_{ij} [S_i S_j - 3r_{ij}^{-2} (S_i r_{ij}) (S_j r_{ij})]. \quad (3)$$

In the above expression: P_{ij} is a pseudodipolar constant equal to P if the sites i and j are the nearest neighbours and equal to 0 in other cases; r_{ij} is the radius vector and S_i is the spin operator assigned to the lattice point i . We define S_F -components in the second quantization representation according to equations

$$\begin{aligned} S_i^X &= \frac{1}{2} (c_i^+ c_{i+} + c_{i+}^+ c_i), \\ S_i^Y &= -\frac{i}{2} (c_i^+ c_{i+} - c_{i+}^+ c_i), \\ S_i^Z &= \frac{1}{2} (c_i^+ c_i - c_{i+}^+ c_{i+}). \end{aligned} \quad (4)$$

Then, H_A can be rewritten as follows

$$\begin{aligned} H_A &= \sum_{i \neq j} \{ D_{ij} (c_i^+ c_i c_j^+ c_j + c_i^+ c_i c_j^+ c_j - \frac{1}{2} c_i^+ c_i c_j^+ c_j - \frac{1}{2} c_i^+ c_i c_j^+ c_j) \\ &\quad + A_{ij} c_i^+ c_i (c_j^+ c_j - c_j^+ c_j) + B_{ij} c_i^+ c_i c_j^+ c_j + \text{h.c.} \}, \end{aligned} \quad (5)$$

where

$$D_{ij} = -\frac{1}{4} P_{ij} \left[1 - 3 \left(\frac{r_{ij}^Z}{r_{ij}} \right)^2 \right], \quad (6)$$

$$A_{ij} = -\frac{3}{8} P_{ij} \frac{r_{ij}^Z (r_{ij}^X - i r_{ij}^Y)}{r_{ij}^2}, \quad (7)$$

$$B_{ij} = -\frac{3}{8} P_{ij} \frac{(r_{ij}^X - i r_{ij}^Y)^2}{r_{ij}^2}. \quad (8)$$

The pseudodipolar Hamiltonian was first introduced by Van Vleck for magneto-crystalline anisotropy investigations [11]. Though such an approach has to some extent a phenomenological character (the coupling constant P is in fact treated as a parameter, which can be determined by experimental data), it was successfully used in the Heisenberg model [1, 12]. As far as the band model is concerned, H_A given by Eq. (5) seems to be the best Hamiltonian consistent with the Hubbard term (2). The pseudodipolar Hamiltonian H_A , describing the interactions between electrons in the Wannier states at two nearest neighbour sites, constitutes a natural complement to the Hubbard model, in which only the intraatomic interactions are taken into account.

Now, by means of the Fourier transformation we transform the Hamiltonian (1) to impulse space and get

$$\begin{aligned} H &= \sum_{k\sigma} \varepsilon_k c_{k\sigma}^+ c_{k\sigma} + \frac{1}{N} \sum_{kk'm} c_{k+m}^+ c_{k'}^+ -_{m1} c_{k'} c_{k1} \\ &\quad \frac{1}{N} \sum_{kk'm} \{ \frac{1}{2} \sum_{\sigma} [D_m (c_{k+m\sigma}^+ c_{k'-m-\sigma}^+ c_{k'\sigma} c_{k-\sigma} - \sum_{\sigma'} \hat{\sigma} \hat{\sigma}' c_{k+m\sigma}^+ c_{k'-m\sigma'}^+ c_{k'\sigma'} c_{k\sigma}) \\ &\quad + \hat{\sigma} A_m c_{k+m}^+ c_{k'}^+ -_{m\sigma} c_{k'\sigma} c_{k1}] + B_m c_{k+m}^+ c_{k'}^+ -_{m1} c_{k'} c_{k1} + \text{h.c.} \}, \end{aligned} \quad (9)$$

where $\hat{\sigma} = \pm 1$, $\varepsilon_k = \sum_i T_{ij} e^{ik(r_i - r)}$ and D_m, A_m, B_m are the Fourier transforms of D_{ij}, A_{ij}, B_{ij} . The form of the Hamiltonian given by Eq. (9) is very convenient and it constitutes a starting point for our calculations. Taking into account that the strength of pseudo-dipolar coupling is small in comparison to intraatomic interaction we will calculate the mean energy of the system and show that this energy depends on the direction of magnetization with respect to the crystal axes. We will find energies and anisotropy constants for crystals of simple cubic and hexagonal lattices. The examples will show that despite the simplicity of our model it is possible to obtain quite reasonable results.

It is worth while to mention that Hamiltonian (9) can be useful for solving problems in which the magnetocrystalline anisotropy plays an important role (e. g. domain structure investigations).

3. Evaluation of anisotropy energy for a crystal of hexagonal structure

For crystals of hexagonal symmetry, because of an uniaxial anisotropy, the free energy density can be expressed in a form

$$F = F_0 + K_1(1 - \alpha_3^2) + K_2(1 - \alpha_3^4) + \dots \quad (10)$$

where K_1 and K_2 are anisotropy constants and α_3 is the direction cosine of the magnetization with respect to hexagonal axis "c". For the Heisenberg model [13] it was pointed out that as far as anisotropy is concerned the entropy contribution of dipolar interactions to the free energy is negligible so the free energy can be approximated by the internal energy of the system. Therefore, in our considerations, we will evaluate the ground state energy as the mean value of the Hamiltonian.

3.1. Simple hexagonal structure

In this section we calculate the mean value of Hamiltonian (9) and derive the anisotropy constant K_1 for simple hexagonal structure. For this purpose we introduce the Green functions $G^{\sigma\sigma'}(k) = \langle\langle c_{k\sigma}; c_{k\sigma'}^+ \rangle\rangle_E$ defined in the standard way [14], which satisfy the equation of motion

$$E \langle\langle c_{k\sigma}; c_{k\sigma'}^+ \rangle\rangle_E = \frac{1}{2\pi} \langle\{c_{k\sigma}, c_{k\sigma'}^+\}\rangle + \langle\langle [c_{k\sigma}, H]; c_{k\sigma'}^+ \rangle\rangle_E. \quad (11)$$

Functions of higher order appearing on the right-hand side of Eq. (11) are decoupled according to the Hartree-Fock procedure and the following set of equations is obtained

$$(E - \varepsilon_k + \hat{\sigma} \varepsilon_k^\Lambda - In_{-\sigma}) G^{\sigma\sigma}(k) = \frac{1}{2\pi} + \mathcal{F}^\sigma(k) G^{-\sigma\sigma}(k), \quad (12)$$

$$(E - \varepsilon_k - \hat{\sigma} \varepsilon_k^\Lambda - In_\sigma) G^{-\sigma\sigma}(k) = \mathcal{F}^{-\sigma}(k) G^{\sigma\sigma}(k), \quad (13)$$

where

$$\varepsilon_k^A = D_0\mu - \frac{1}{N} \sum_{m\sigma'} \hat{\sigma}' D_m n_{k+m\sigma'}, \quad (14)$$

$$\mathcal{F}^\sigma(\mathbf{k}) = \hat{\sigma}(A_0\delta_{\sigma\uparrow} + A_0^*\delta_{\sigma\downarrow})\mu + \frac{1}{N} \sum_m (A_m\delta_{\sigma\uparrow} + A_m^*\delta_{\sigma\downarrow}) \left(\sum_{\sigma'} n_{k+m\sigma'} - 1 \right), \quad (15)$$

$$n_\sigma = \frac{1}{N} \sum_k n_{k\sigma} = \frac{1}{N} \sum_k \langle c_{k\sigma}^+ c_{k\sigma} \rangle, \quad (16)$$

$$\mu = \sum_\sigma \hat{\sigma} n_\sigma, \quad (17)$$

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

Then, one-electron Hartree-Fock energies are given by

$$E_k^s = \varepsilon_k + \frac{1}{2} I n - \frac{\hat{s}}{2} \Delta_k, \quad (18)$$

$$\Delta_k = [(I\mu + 2\varepsilon_k^A)^2 + 4\mathcal{F}^\sigma(\mathbf{k})\mathcal{F}^{-\sigma}(\mathbf{k})]^{1/2}, \quad (19)$$

and $\hat{s} = +1$ or -1 . Let us pay attention to the fact that the presence of pseudodipolar coupling leads to a modification of the energy gap between spin-split bands. We can see (Eq. (19)) that the energy gap depends on the wave vector k , so the splitting is different in various points of the Brillouin zone.

The internal energy of the crystal (the mean value of Hamiltonian (9)) is equal to

$$E = \sum_{ks} E_k^s f(E_k^s) - \frac{N}{4} (I + D_0) (n^2 - \mu^2) + \frac{N}{4} D_0 (n^2 + \mu^2) - \frac{\mu}{2} \sum_m D_m \left[1 + \frac{1}{N} \sum_{k\sigma} (n_{k\sigma} - n_{k-\sigma}) n_{k+m\sigma} \right], \quad (20)$$

where

$$n = \frac{1}{N} \sum_{ks} f(E_k^s), \quad (21)$$

$$\mu = \frac{1}{N} \sum_{ks} \frac{I\mu + 2\varepsilon_k^A}{\Delta_k} \hat{s} f(E_k^s). \quad (22)$$

In the above expressions $f(E_k^s)$ represents the Fermi-Dirac distribution function.

Equations (20)–(22) constitute a self-consistent set. To solve this set we introduce some approximations. Since, the pseudodipolar coupling constant P is much smaller than I —the parameter of intraatomic Coulomb interaction—we can expand expression (19) into a power series for P/I and neglect all terms of higher order than P/I . We assume also that the distribution function of occupation numbers for one-electron Hartree-Fock states is the same as for an isotropic ferromagnet, i.e., $f(E_k^{\sigma}) \simeq f(E_k^{0\sigma})$. Then, the mean energy of the system is equal to

$$E = \sum_{k\sigma} \varepsilon_k f(E_k^{0\sigma}) + \frac{N}{4} (n^2 - \mu_0^2) - \frac{N}{2} D_0 \mu_0^2 + \frac{1}{2N} \sum_{\substack{km \\ \sigma\sigma'}} \hat{\sigma} \hat{\sigma}' D_{m-k} f(E_k^{0\sigma}) f(E_m^{0\sigma'}), \quad (23)$$

where

$$\mu_0 = \frac{1}{N} \sum_{k\sigma} f(E_k^{0\sigma}).$$

Energy E depends on the direction of the magnetization vector with respect to the crystallographic axes through D_0 and D_m which in turn are related to the pseudodipolar interaction. According to Eq. (6)

$$D_0 = \sum_h D_h = -\frac{1}{4} \sum_h P_h \left[1 - 3 \left(\frac{r_h^z}{r_h} \right)^2 \right], \quad (24)$$

where $r_h = |r_i - r_j|$ is the radius vector to nearest neighbours, and its components r_h^i ($i = X, Y, Z$) are taken with respect to quantization axes. To obtain the anisotropy constant, it is necessary to transform the components of r_h to crystal axes by use of the relation: $r_h^i = \sum_i \alpha_{i1} r_h^i$, where α_{i1} are the direction cosines and $i = x, y, z$. Taking the sum over the nearest neighbours, we obtain

$$D_0 = \frac{1}{4} (3P_1 - 2P_2) [-2 + 3(1 - \alpha_3^2)]. \quad (25)$$

P_1 and P_2 denote here the pseudodipolar coupling constants, and $P_h = P_1$ if the considered sites are from the same hexagonal plane or $P_h = P_2$ if they are from adjacent planes and $\alpha_3 = \alpha_{z1}$.

In order to calculate the last term in Eq. (23) we use the inverse Fourier transformation and define functions b_h

$$b_h = \frac{1}{N^2 \mu_0^2} \sum_{\substack{km \\ \sigma\sigma'}} \hat{\sigma} \hat{\sigma}' e^{i(m-k)r_h} f(E_k^{0\sigma}) f(E_m^{0\sigma'}). \quad (26)$$

It allows us to express the considered term as a sum over the nearest neighbours in a direct lattice of the type $\sum_h D_h b_h$. Taking into account the crystal symmetry and using the same procedure as for the calculation of D_0 , we get

$$\sum_h D_h b_h = \frac{1}{4} (3P_1 b_{100} - 2P_2 b_{001}) [-2 + 3(1 - \alpha_3^2)]. \quad (27)$$

After that, we can find the anisotropy constant K_1 . It is given by the formula

$$K_1 = \frac{3\mu_0^2}{8V_0} [2P_2(1-b_{001})-3P_1(1-b_{100})], \quad (28)$$

where V_0 is the volume of the primitive cell.

3.2. Hexagonal-close-packed structure

In hexagonal-close-packed lattice there are two atoms in the elementary cell, so the lattice can be treated as consisting of two equivalent and interacting sublattices of simple hexagonal structure. Then, Hamiltonian (9), which constitutes a base for our calculations, should be rewritten in a different form including the presence of two sublattices, namely

$$\begin{aligned} H = & \sum_{k\sigma} \sum_{\alpha\beta} \varepsilon_k^{\alpha\beta} c_{k\alpha\sigma}^+ c_{k\beta\sigma} + \frac{I}{N} \sum_{kk'm} \sum_{\alpha} c_{k+m\alpha}^+ c_{k'-m\alpha}^+ c_{k'\alpha} c_{k\alpha} \\ & + \frac{1}{N} \sum_{kk'm} \sum_{\alpha\beta} \left\{ \frac{1}{2} \sum_{\sigma} [D_m^{\alpha\beta} (c_{k+m\alpha\sigma}^+ c_{k'-m\beta-\sigma}^+ c_{k'\beta\sigma} c_{k\alpha-\sigma} - \sum_{\sigma} \hat{\sigma} \hat{\sigma}' c_{k+m\alpha\sigma}^+ c_{k'-m\beta\sigma}^+ c_{k'\beta\sigma} c_{k\alpha\sigma}) \right. \\ & \left. + \hat{\sigma} A_m^{\alpha\beta} c_{k+m\alpha}^+ c_{k'-m\beta\sigma}^+ c_{k'\beta\sigma} c_{k\alpha} \right] + B_m^{\alpha\beta} c_{k+m\alpha}^+ c_{k'-m\beta}^+ c_{k'\beta} c_{k\alpha} + \text{h.c.} \left. \right\}. \quad (29) \end{aligned}$$

In Hamiltonian (29) $\varepsilon_k^{\alpha\beta} = \sum_i T_{ij}^{\alpha\beta} e^{ik(r_i-r_j)}$, where $T_{ij}^{\alpha\beta}$ denote hopping integrals from the point i of sublattice α to its nearest neighbour j in sublattice β and $D_m^{\alpha\beta}$, $A_m^{\alpha\beta}$, $B_m^{\alpha\beta}$ are the Fourier transforms of $D_{ij}^{\alpha\beta}$, $A_{ij}^{\alpha\beta}$, $B_{ij}^{\alpha\beta}$. N denotes number of elementary cells and α, β are equal to 1 or 2.

We calculate the mean energy of the system by using the Green function formalism. We introduce the functions: $G_{\alpha\beta}^{\sigma\sigma'}(k) = \langle\langle c_{k\alpha\sigma}; c_{k\beta\sigma'}^+ \rangle\rangle_E$ and in the Hartree-Fock approximation, taking into account that the pseudodipolar coupling constant is small in comparison with the parameter of intraatomic Coulomb interaction as well as to the bandwidth, we get for one-electron energies the following formula

$$\begin{aligned} E_{k\eta}^{\sigma} = & \varepsilon_k + I n_{-\sigma} - \hat{\sigma} \left[\mu_0 (D_0 + D_0^{12}) - \frac{1}{N} \sum_{m\sigma'} \hat{\sigma}' D_m n_{k-m\sigma'} \right] \\ & - \frac{\hat{\eta}}{2} \left(\sqrt{\varepsilon_k^{12} \varepsilon_k^{21}} + \hat{\sigma} \sqrt{\frac{\varepsilon_k^{12}}{\varepsilon_k^{21}}} D^{21}(\mathbf{k}) + \hat{\sigma} \sqrt{\frac{\varepsilon_k^{21}}{\varepsilon_k^{12}}} D^{12}(\mathbf{k}) \right), \quad (30) \end{aligned}$$

where

$$D^{12}(\mathbf{k}) = \frac{1}{2N} \sum_{m\sigma'} D_m^{21} \hat{\sigma}' \langle c_{k-m1\sigma'}^+ c_{k-m2\sigma'} \rangle, \quad (31)$$

and

$$\langle c_{k1\sigma}^+ c_{k2\sigma} \rangle = \frac{1}{2} \sqrt{\frac{\varepsilon_k^{21}}{\varepsilon_k^{12}}} \sum_{\eta} \hat{\eta} f(E_{k\eta}^{\sigma}). \quad (32)$$

$f(E_{k\eta}^\sigma)$ represents here the Fermi-Dirac distribution function and $\hat{\eta} = +1$ or -1 . Since both sublattices are equivalent in formula (30) we set: $n_{k\alpha\sigma} \equiv n_{k\sigma}$, $\mu_\alpha \equiv \mu$, $\varepsilon_k^{\alpha\alpha} \equiv \varepsilon_k$ and $D_m^{\alpha\alpha} \equiv D_m$.

Next, we assume that the distribution function of occupation numbers for one-electron Hartree-Fock states is the same as for an isotropic ferromagnet, i.e., $f(E_{k\eta}^\sigma) \simeq f(E_{k\eta}^{0\sigma})$ and calculate the mean energy of the system. We obtain

$$E = \sum_{k\sigma\eta} \varepsilon_k f(E_{k\eta}^{0\sigma}) + \frac{N}{2} I(n^2 - \mu_0^2) + \frac{1}{2} \sum_{k\sigma\eta} \hat{\eta} \sqrt{\varepsilon_k^{12} \varepsilon_k^{21}} f(E_{k\eta}^{0\sigma}) - \mu_0^2 N (D_0 + D_0^{12}) + \frac{1}{N} \sum_{\substack{km \\ \sigma\sigma'\eta\eta'}} \hat{\sigma}\hat{\sigma}' D_{m-k} f(E_{k\eta}^{0\sigma}) f(E_{m\eta'}^{0\sigma'}), \quad (33)$$

where

$$\mu_0 = \frac{1}{2N} \sum_{k\eta\sigma} \hat{\sigma} f(E_{k\eta}^{0\sigma}).$$

We can find the anisotropy constant K_1 in the same way as in Sec. 3.1. Namely, we represent D_0, D_m in formula (33) through the components of the radius vector r_h expressed with respect to crystallographic axes and we take a summation over the nearest neighbour sites in a hexagonal-close-packed lattice. It leads to the result

$$K_1 = \frac{9\mu_0^2}{4V_0} \left[P_1(b_{100} - 1) + \frac{6\gamma^2 - 4}{4 + 3\gamma^2} P_2 \right], \quad (34)$$

where function b_h is defined as follows

$$b_h = \frac{1}{4N^2\mu_0^2} \sum_{\substack{km \\ \sigma\sigma'\eta\eta'}} \hat{\sigma}\hat{\sigma}' e^{i(m-k)r_h} f(E_{k\eta}^{0\sigma}) f(E_{m\eta'}^{0\sigma'}) \quad (35)$$

and $\gamma^2 = c/a$ (c, a — the lattice constants).

We can conclude that for hexagonal structures, the anisotropy constant K_1 can be easily calculated by means of the presented method. It should be emphasized that such parameters of the band structure as the Fermi level position in the band and occupation numbers of one-electron Hartree-Fock states (through function b_{100}) essentially influence K_1 .

Expression (34) allows one to draw some simple conclusions concerning the temperature dependence of the anisotropy constant. In this expression the magnetization μ_0 , the parameter γ and function b_{100} (through variation of occupation numbers and shifting of the Fermi level) are related to temperature. An increase in temperature will lead to a decrease in the K_1 constant.

4. Evaluation of anisotropy energy for a crystal of cubic structure

In this section we use Hamiltonian (9) to calculate anisotropy energy for cubic symmetry. The energy density for such crystals can be expressed as follows

$$E = E_0 + K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_1^2\alpha_3^2) + K_2\alpha_1^2\alpha_2^2\alpha_3^2 + \dots \quad (36)$$

where α_i are the direction cosines of the magnetization with respect to the crystallographic axes.

For cubic crystals the energy of the system, in the Hartree-Fock approximation, does not exhibit anisotropy. In this case, because of the cubic symmetry, the pseudodipolar Hamiltonian does not give rise to anisotropy in the first order of the perturbation theory. Therefore, the calculations should be carried out more accurately and higher orders of the perturbation theory are necessary. For this purpose we suggest using the spin wave method. The method allows one to find a microscopic formula for the constant K_1 as well as to determine its temperature dependence. Such an approach was successfully used for analogical investigations in the Heisenberg model [1, 12].

To calculate the mean energy of the system, we express Hamiltonian (9) in terms of creation and annihilation operators of magnons, which are denoted by β_q^+ and β_q , respectively. We use the effective Hamiltonian method, the concept of which has been introduced by Morkowski [15] to investigate spin waves in the presence of pure dipolar interactions within the framework of the band model. The method has been used for examining many-magnon processes and the obtained results have been in good agreement with other theories and experimental data [16, 17].

The effective Hamiltonian with terms up to the fourth order in the magnon operators takes the form

$$\begin{aligned} H_e = & \sum_q \{K_q(\beta_q^+\beta_q + \frac{1}{2}) + L_q\beta_q\beta_{-q} + \text{h.c.}\} + \sum_{qq'} (C_{qq'}\beta_{q+a'}^+\beta_q\beta_{q'} + \text{h.c.}) \\ & + \sum_{qq'a''} (F_{qa'a''}\beta_{q+a'+a''}^+\beta_q\beta_{q'}\beta_{q''} + \text{h.c.}) + \sum_{kk'q} \Gamma_{kk'q}^q \beta_{k+a}^+\beta_{k'-a}\beta_k\beta_{k'}. \end{aligned} \quad (37)$$

We assume that the Hamiltonian H_e (Eq. (37)) is equivalent to our basic Hamiltonian H (Eq. (9)) in the same sense as in paper [15], i. e., the coefficients are defined by

$$\begin{aligned} K_q &= \langle [\beta_q, [H, \beta_q^+]] \rangle, \\ L_q &= \frac{1}{2} \langle [[H, \beta_q^+], \beta_{-q}^+] \rangle, \\ C_{qq'} &= \frac{1}{2} \langle [\beta_{q+a'}, [[H, \beta_q^+], \beta_{q'}^+]] \rangle, \end{aligned} \quad (38)$$

and analogically for higher order terms. The averages $\langle \dots \rangle$ are taken over the Hubbard Hamiltonian ground state and β_q^+ operators are defined according to formula

$$\beta_a^+ = \sum_k b_{k+a,k} c_{k+a}^+ c_{k\uparrow}, \quad (39)$$

The coefficients $b_{k+q,k}$ are normalized to satisfy the boson commutation relation. Then

$$b_{k+q,k} = \frac{d_q}{\varepsilon_{k+q} - \varepsilon_k + \Delta - \hbar\omega_q^0}, \quad (40)$$

where

$$|d_q| = \left\{ \sum_k \frac{n_k}{(\varepsilon_{k+q} - \varepsilon_k + \Delta - \hbar\omega_q^0)^2} \right\}^{-1/2}, \quad (41)$$

and $\Delta = In \cdot \hbar\omega_q^0$ denotes here the spin energy in the absence of the pseudodipolar coupling. It can be found from the condition

$$\frac{I}{N} \sum_k \frac{n_k}{\varepsilon_{k+q} - \varepsilon_k + \Delta - \hbar\omega_q^0} = 1. \quad (42)$$

The above expressions are valid for the case of a strong ferromagnet, i. e., when all states with spin down are empty. We will consider this case only.

Calculating the coefficients in H_e according to formula (38) we obtain

$$K_q = \hbar\omega_q^0 + D_q N (d_q/I)^2 - N^{-1} \sum_{kk'} D_{k'} [|b_{k+q,k}|^2 n_k (n_{k+k'} + n_{k+k'+q}) + b_{k+q,k} b_{k+k'+q,k+k'}^* n_k n_{k+k'}], \quad (43)$$

$$L_q = B_q (d_q/I)^2 N - N^{-1} \sum_{kk'} B_{k'} b_{k+k',k+k'+q} n_k n_{k+k'+q}, \quad (44)$$

$$C_{qq'} = \frac{1}{2} (\bar{C}_{qq'} + \bar{C}_{q'q}), \quad (45)$$

$$\begin{aligned} \bar{C}_{qq'} = & -A_q N^{-1} \sum_{kk'} b_{k+q,k} b_{k'+q+q',k'}^* (b_{k'+q',k'} + b_{k'+q+q',k'+q}) n_k n_{k'} \\ & + N^{-1} \sum_{kk'} A_{k'} b_{k+q,k} b_{k'+q+q',k}^* (b_{k'+q+q',k+q} + b_{k+k'+q+q',k+k'+q}) n_k n_{k+k'+q} \\ & + N^{-1} \sum_{kk'} A_{k'} b_{k+q+q',k+q} b_{k+k'+q',k+k'} b_{k'+q+q',k}^* n_k n_{k+k'}, \end{aligned} \quad (46)$$

$$F_{qq'a'} = \frac{1}{2} (\bar{F}_{qq'a'} + \bar{F}_{q'a'q} + \bar{F}_{a'qa'}), \quad (47)$$

$$\begin{aligned} \bar{F}_{qq'a'} = & -B_q N^{-1} \sum_{kk'} b_{k+q,k} b_{k'+q',k'} b_{k'+q+q'+a'',k'+q+q'} b_{k'+q+q'+a'',k}^* n_k n_{k'} \\ & - B_{q'} N^{-1} \sum_{kk'} b_{k+q,k} b_{k'+q',k'} b_{k'+q+q'+a'',k+q+a'} b_{k'+q+q'+a'',k}^* n_k n_{k'} \\ & + N^{-1} \sum_{kk'} B_{k'-k-a} b_{k+q,k} b_{k'+q',k'} b_{k'+q+q'+a'',k+q+a'} b_{k'+q+q'+a'',k}^* n_k n_{k'} \\ & + N^{-1} \sum_{kk'} B_{k'-k-a} b_{k+q',k} b_{k'+q,k} b_{k'+q+q'+a'',k+q+a'} b_{k'+q+q'+a'',k}^* n_k n_{k'}, \end{aligned} \quad (48)$$

where D_q, A_q, B_q are the Fourier transforms of expressions (6)–(8). It is easy to see that the coefficients in H_e depend on the band structure of a ferromagnet and on the occupation numbers of one-electron states.

The contribution to the mean energy of the system, arising from the pseudodipolar Hamiltonian, is evaluated by means of the perturbation theory. We neglect the influence of the last term in H_e , Eq. (37), which describes spin waves interaction (that is why the expressions for $\Gamma_{kk'}^q$ has been omitted). The neglecting of these interactions seems to be completely justified at low temperatures, at which only a low number of magnons is excited. We carry out the calculations to the second order of perturbation and get the following contribution to the energy

$$\Delta E = -2 \sum_q \frac{|L_q|^2}{\hbar\omega_q^0} (N_q + \frac{1}{2}) - 3 \sum_{q,q'} \frac{L_q F_{q-q'}^* + L_{q'}^* F_{q-q'}}{\hbar\omega_q^0} N_{q'} - \sum_q \frac{|C_{q-q}|^2}{\hbar\omega_q^0} \sum_{q'} N_{q'}, \quad (49)$$

where N_q denote magnon state occupation numbers. The expression ΔE depends on the direction of magnetization with respect to the crystal axes through coefficients L_q , $C_{qq'}$ and $F_{qq'q''}$ which are connected with pseudodipolar coupling. However, in general, we are not able to express ΔE , given by Eq. (49), in a form like Eq. (36) and to calculate the anisotropy constant K_1 . To solve the problem, it is necessary to determine the band structure and moreover, to introduce some simplifications. We assume a parabolic shape for the electron energy band and we assume also that the main contributions to the coefficients L_q , $C_{qq'}$ and $F_{qq'q''}$ are caused by long spin waves. This allows us to expand expressions (44), (46) and (48) into a power series with respect to q and to neglect terms of higher order than q^2 . Such a procedure is valid for low temperatures. We neglect also the dependence of one-electron state occupation numbers on q .

Taking into account the above approximations as well as the crystal symmetry we obtain for anisotropy energy of simple cubic lattice a formula

$$E_{\text{anis}} = \frac{9n^2 NP^2}{16} \left\{ v - \chi^2 k_F^2 \left(\frac{2}{3} \omega + 4\mu - 2\kappa \right) - [24v - 40\omega \left(\frac{2}{3} \chi^2 k_F^2 - \frac{1}{2} \chi \right) - \chi^2 k_F^2 (116\mu - 48\kappa)] \frac{1}{nN} \sum_q N_q \right\} (\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_1^2 \alpha_3^2), \quad (50)$$

where P is the pseudodipolar coupling constant, n — the mean number of electrons per atom, k_F — the Fermi momentum and $\chi = \hbar^2/m^* \Delta$ (m^* — the effective mass). Besides, we have introduced the following notations

$$\omega = a_{000} + a_{200} - 2a_{110}, \quad (51)$$

$$v = b_{000} + b_{200} - 2b_{110}, \quad (52)$$

$$\mu = 2(c_{100,100} - c_{100,010}), \quad (53)$$

$$\kappa = 2(d_{100,100} - d_{100,010}), \quad (54)$$

where

$$a_h = \frac{1}{N} \sum_q q^2 (\hbar\omega_q^0)^{-1} e^{iqr_h}, \quad (55)$$

$$b_h = \frac{1}{N} \sum_q (\hbar\omega_q^0)^{-1} e^{iqr_h}, \quad (56)$$

$$c_{h_1, h_2} = \frac{1}{n^2 N^3 k_F^2} \sum_{qkk'} (\hbar\omega_q^0)^{-1} (kq)^2 e^{i[qr_{h_1} + (k'-k)r_{h_2}]} n_k n_{k'}, \quad (57)$$

$$d_{h_1, h_2} = \frac{1}{n^2 N^3 k_F^2} \sum_{qkk'} (\hbar\omega_q^0)^{-1} (kq) (k'q) e^{i[qr_{h_1} + (k'-k)r_{h_2}]} n_k n_{k'} \quad (58)$$

and r_h is the radius vector to the nearest neighbours.

The anisotropy constant

$$K_1 = \frac{9n^2 P^2}{16V_0} \left\{ v - \chi^2 k_F^2 \left(\frac{2}{3} \omega + 4\mu - 2\kappa \right) - [24v - 40\omega \left(\frac{2}{3} \chi^2 k_F^2 - \frac{1}{2} \chi \right) - \chi^2 k_F^2 (116\mu - 48\kappa)] \frac{1}{nN} \sum_q N_q \right\} \quad (59)$$

is calculated here for the case of a simple cubic lattice only. The derivation of analogous expressions for other cubic lattices does not present any difficulties.

According to formula (59), the constant K_1 essentially depends on such parameters as the energy gap, the Fermi energy and effective mass. Moreover, by means of coefficients c_{h_1, h_2} and d_{h_1, h_2} , K_1 depends on the position of the Fermi level in the band. The strong dependence of the anisotropy constant on the Fermi level position was also mentioned in other theoretical papers, in which more accurate approaches were used [8].

It should be emphasized that it is possible to perform more accurate calculations within the framework of the discussed model. For this purpose, first of all, more realistic band structures should be taken into account. However, for such structures numerical calculations would be necessary, so we could not obtain any analytical expression for the anisotropy constant. The calculations would allow us to estimate the constant K_1 and to compare the results with experimental data.

We want to mention that, in literature, despite the use of more and more complicated theoretical models in which not only real band structures but also many other effects (the deformation of the Fermi surface caused by spin-orbit interaction, the existence of degenerate bands near the Fermi level and so on) have been taken into account, complete agreement between theoretical and experimental data concerning the anisotropy constant K_1 for transition metals and especially for nickel has not been achieved. To some extent, the discrepancy can be due to the fact that the anisotropy constant K_1 is determined theoret-

cally from the expansion of free energy into a power series when constant strains are assumed. On the other hand, the experimental measurements are usually performed under conditions of constant external stresses. Therefore, to compare the results, one should take into account those corrections which can appear to be important.

The temperature dependence of the anisotropy constant K_1 has been investigated within the framework of the band model rather seldom [8, 9]. According to our considerations, it is clear that there are several agents which influence the temperature variation of anisotropy. First of all, the spin waves cause a decrease in the constant K_1 with increasing temperature. Then, the variation of the distribution function of one-electron occupation numbers as well as a displacement of the Fermi level influence also the temperature dependence of K_1 constant.

On the basis of these qualitative considerations, we can find that K_1 depends on temperature in a different way than in the Heisenberg model [1]. Whereas calculations performed using the spin wave method in the localized spin model lead to a well-known power law, in our case, within the framework of the band model, the temperature dependence of the anisotropy constant has a more complicated character.

5. Summary

In this paper we have presented, within the framework of the band model, the theory of magnetocrystalline anisotropy, based on the pseudodipolar Hamiltonian. The calculations have been performed for the simple cubic and hexagonal lattices. We have shown that the considered method allows one to obtain the anisotropy constants as functions of the band parameters (the energy gap, the Fermi energy). On the basis of the derived expressions it is possible to draw some conclusions concerning the temperature dependence of anisotropy constants. Rough qualitative considerations show that this dependence does differ from the power law.

The obtained results constitute evidence that the pseudodipolar Hamiltonian can be successfully used within the framework of the band model for describing the magnetocrystalline anisotropy in all problems in which anisotropy is important and other methods are ineffective. One of the examples is an investigation of domain structure. We will undertake this problem in a separate paper.

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