

THE INFLUENCE OF THE TEMPERATURE ON THE BLOCH WALL THICKNESS

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By applying the Heisenberg model and Bogolubov's variational method in the molecular field approximation (MFA) to three-axial ferromagnets with $(90^\circ|90^\circ)$ Bloch walls, a temperature dependent equation for the domain structure is derived and the dependence of the Bloch wall thickness on the temperature is examined. The results are illustrated by numerical calculations.

1. Introduction

The thermodynamic behaviour of ferromagnets at high temperatures was investigated theoretically as well as experimentally in numerous papers. None the less, it can hardly be said that this problem has been solved completely. This is especially true for the case of ferromagnets with domain structures, as in nearly all theoretical investigations the existence of domains has been neglected. The lack of adequate experimental data is one of the main reasons for the present situation. There are only a few papers in which, *e.g.*, the widening [1] and vanishing [2] of Bloch walls below the Curie temperature had been established.

Recently, we studied in a series of papers [3]–[7] the transition of a ferromagnet with domain structure to the paramagnetic state by applying Bogolubov's inequality and the MFA method.

Under the assumption that the domain structure exists up to the conventional transition temperature, the notion of a local transition temperature was introduced and shown to vary within the structure, being largest at domain centres and smallest in the interdomain walls [3].

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This effect was shown to exist in ferromagnets and in two-sublattice antiferromagnets with 180° interdomain walls. The results imply that the transition of a magnetic crystal with domain structure to the paramagnetic state takes place in a certain temperature interval rather than at a sharply defined temperature. The local transition temperatures which form this interval determine the singularities of the second derivative of the partition function [4]. In paper [6], a relationship between the width of the transition temperature interval and the Bloch wall energy density was established, and in [7] a crystal with monoionic anisotropy was examined. The same problem was solved in [8] by using the Green function and Wallace's method instead of the MFA method. All the results mentioned above were obtained for uniaxial magnets only.

The purpose of the present paper is to extend the considerations to ferromagnets with three-axial anisotropy. We examine only one type of domain structure, namely, a structure composed of $(90^\circ|90^\circ)$ Bloch walls. In the second part of the paper, the temperature dependence of the $(90^\circ|90^\circ)$ Bloch wall thickness is derived.

2. Derivation of the thermodynamic equilibrium equation

We start with the Hamiltonian

$$H = -\frac{1}{2} \sum_{fg} P_{fg}^{\alpha\beta} S_f^\alpha S_g^\beta - \sum_{fg} Q_{fg}^{\alpha\beta\gamma\delta} S_f^\alpha S_f^\beta S_g^\gamma S_g^\delta, \quad (1)$$

where S_f^α is the α -component of the spin operator at the lattice site f . Throughout the paper, expect where stated otherwise, Einstein's summation rule is applied to the tensor indices α, β . The spin components satisfy the standard commutation relations. Here, the tensor $P_{fg}^{\alpha\beta}$ describes isotropic interactions only, and the tensor $Q_{fg}^{\alpha\beta\gamma\delta}$ represents anisotropic interactions. They can be specified as follows:

$$P_{fg}^{\alpha\beta} = J_{fg} \delta_{\alpha\beta}, \quad (2)$$

$$Q_{fg}^{\alpha\beta\gamma\delta} = \frac{1}{2} K \delta_{fg} \delta^{\alpha\beta} \delta^{\gamma\delta} (1 - \delta^{\alpha\delta}). \quad (3)$$

The Hamiltonian (1) with the interaction tensors (2) and (3) describes a ferromagnetic crystal of cubic symmetry. Actually, from the microscopical point of view the tensor (3) no longer represents an interaction, but merely a sort of anisotropic self-energy [9].

We shall use Bogolubov's inequality for the free energy (see, e.g., [10])

$$F(H) \leq F_{\text{mod}}(H) = -\frac{1}{\beta} \ln \text{Tr} e^{-\beta H_0} + \frac{\text{Tr} (H - H_0) e^{-\beta H_0}}{\text{Tr} e^{-\beta H_0}} \quad (4)$$

where

$$H_0 = -\sum_f M_f^\alpha S_f^\alpha \quad (4a)$$

and $\beta^{-1} = kT$.

To calculate $F_{\text{mod}}(H)$ we introduce the local coordinate system

$$M_f^\alpha S_f^\alpha = M_f n_f^\alpha S_f^\alpha = M_f S_f^n. \quad (5)$$

Then, it can easily be shown that

$$\text{Tr } e^{-\beta H_0} = \prod_f \frac{\text{sh } \beta M_f \left(S + \frac{1}{2} \right)}{\text{sh } \frac{1}{2} \beta M_f} \equiv \prod_f Z_f. \quad (6)$$

In order to obtain the right-hand side of Eq. (4) we need to calculate the averages $\langle S_f^\alpha S_g^\beta \rangle_0$ and $\langle S_f^\alpha S_f^\beta S_g^\gamma S_g^\delta \rangle_0$ where

$$\langle \dots \rangle_0 \equiv \frac{\text{Tr } \dots e^{-\beta H_0}}{\text{Tr } e^{-\beta H_0}}. \quad (7)$$

The basic quantity characterizing a magnetic crystal is apparently the magnetization vector $\vec{\sigma}_f$ defined as follows:

$$\sigma_f^\alpha \equiv \langle S_f^\alpha \rangle_0. \quad (8)$$

According to Eqs (5), (6) and (7) we have (see [3])

$$\sigma_f^\alpha = n_f^\alpha B(\beta M_f), \quad (9)$$

where

$$B(\beta M_f) = \left(S + \frac{1}{2} \right) \text{cth} \left(S + \frac{1}{2} \right) \beta M_f - \frac{1}{2} \text{cth} \frac{1}{2} \beta M_f$$

and

$$\langle S_f^\alpha S_g^\beta \rangle_0 = \sigma_f^\alpha \sigma_g^\beta = n_f^\alpha n_g^\beta B(\beta M_f) B(\beta M_g). \quad (10)$$

To calculate the average $\langle \sum_f Q_{ff}^{\alpha\beta\gamma\delta} S_f^\alpha S_f^\beta S_f^\gamma S_f^\delta \rangle_0$ we carry out the transformation of the spin operators to the local coordinate system

$$\begin{aligned} S_f^\alpha &= \sum_\sigma a_{\alpha\sigma} S_f'^\sigma, & S_f^\beta &= \sum_\rho a_{\beta\rho} S_f'^\rho, \\ S_f^\gamma &= \sum_\tau a_{\gamma\tau} S_f'^\tau, & S_f^\delta &= \sum_\xi a_{\delta\xi} S_f'^\xi, \end{aligned}$$

where $a_{\alpha\sigma}$ — are elements of the transformation matrices. The local coordinate system denoted by primes is chosen in such a way that the x'_3 axis is parallel to the vector \vec{M}_f . Then,

$$\langle \sum_f Q_{ff}^{\alpha\beta\gamma\delta} S_f^\alpha S_f^\beta S_f^\gamma S_f^\delta \rangle_0 = \langle \sum_f Q'_{ff}{}^{\sigma\rho\tau\xi} S_f'^\sigma S_f'^\rho S_f'^\tau S_f'^\xi \rangle_0 \equiv \langle A \rangle_0, \quad (11)$$

where

$$Q'_{ff}{}^{\sigma\rho\tau\xi} = \sum_{\alpha\beta\gamma\delta} Q_{ff}^{\alpha\beta\gamma\delta} a_{\alpha\sigma} a_{\beta\rho} a_{\gamma\tau} a_{\delta\xi}.$$

Upon passing from the operators $S_f^{\prime\sigma}$ to the operators $S_f^{\prime+}, S_f^{\prime-}, S_f^{\prime3}$ and taking into account the relations between $S_f^{\prime+}S_f^{\prime-}$ and $S_f^{\prime3}$ as well as Eq. (3) we get, after somewhat tedious calculations, the following equation:

$$\langle A \rangle_0 = \frac{1}{8} K \sum_f \left\{ 2S(S+1) + S^2(S+1)^2 + W(\sigma_f) - \frac{1}{2} \sum_{\alpha \neq \beta} (n_f^\alpha)^2 (n_f^\beta)^2 [6S(S+1) - 3S^2(S+1)^2 + 5W(\sigma_f)] \right\}, \tag{12}$$

where

$$W(\sigma_f) = [6S(S+1) - 5] \langle S_f^{\prime3} \rangle_0 - 7 \langle S_f^{\prime3} \rangle_0^4 \tag{12a}$$

(see Appendix I), and n_f^α are the direction cosines of the x'_3 axis of the local coordinate system with respect to the previous coordinate system.

In the local coordinate system we have, according to (5),

$$H_0 = - \sum_f M_f S_f^{\prime3}. \tag{13}$$

By the use of Eq. (7) it can easily be shown that

$$\begin{aligned} \langle (S_f^{\prime3})^{n+1} \rangle_0 &= \frac{\partial}{\partial \beta M_f} \frac{\text{Tr} (S_f^{\prime3})^n e^{-\beta H_0}}{\text{Tr} e^{-\beta H_0}} = \frac{\partial}{\partial \beta M_f} \frac{\text{Tr} (S_f^{\prime3})^n e^{-\beta H_0}}{\text{Tr} e^{-\beta H_0}} + \\ &+ \frac{(\text{Tr} (S_f^{\prime3})^n e^{-\beta H_0})(\text{Tr} S_f^{\prime3} e^{-\beta H_0})}{(\text{Tr} e^{-\beta H_0})^2} = \left\{ \frac{\partial}{\partial \beta M_f} + \langle S_f^{\prime3} \rangle_0 \right\} \cdot \langle (S_f^{\prime3})^n \rangle_0, \end{aligned} \tag{14}$$

for $n = 1, 2, \dots$, and by taking into account Eq. (8) we have

$$\langle (S_f^{\prime3})^m \rangle_0 = \left(\frac{\partial}{\partial \beta M_f} + \sigma_f \right)^{m-1} \sigma_f \tag{15}$$

for $m = 1, 2, 3, \dots$ Finally, we obtain for the model free-energy the following expression:

$$\begin{aligned} F_{\text{mod}}(H) &= - \frac{1}{\beta} \sum_f \ln Z_f + \sum_f M_f^\alpha \sigma_f^\alpha - \frac{1}{2} \sum_{f \neq g} P_{fg}^{\alpha\beta} \sigma_f^\alpha \sigma_g^\beta - \frac{1}{8} K \sum_f \left\{ 2S(S+1) + \right. \\ &\left. + S^2(S+1)^2 + W(\sigma_f) - \frac{1}{2} \sum_{\alpha \neq \beta} (n_f^\alpha)^2 (n_f^\beta)^2 [6S(S+1) - 3S^2(S+1)^2 + 5W(\sigma_f)] \right\}. \end{aligned} \tag{16}$$

According to the MFA method, we minimize F_{mod} with respect to the parameters M_f and n_f^α taking into consideration the condition $n_f^\alpha n_f^\alpha = 1$. This leads to the equations

$$\frac{\partial \sigma}{\partial \beta M_f} \left(M_f - \sum_{g(\neq f)} J_{fg} n_f^\alpha \sigma_g^\alpha \right) = \frac{1}{8} K \frac{\partial W(\sigma_f)}{\partial \beta M_f} \left\{ 1 - \frac{5}{2} \sum_{\alpha \neq \beta} (n_f^\alpha)^2 (n_f^\beta)^2 \right\}, \quad (17)$$

$$\sigma_f \sum_{g(\neq f)} J_{fg} \sigma_g^\alpha + \frac{1}{4} K n_f^\alpha [1 - (n_f^\alpha)^2] [3S^2(S+1)^2 - 6S(S+1) - 5W(\sigma_f)] = \lambda_f n_f^\alpha. \quad (18)$$

In the above formulae, the summation rule for the tensor indices α, β does not apply.

3. Ferromagnet with domain structure

We consider a ferromagnet with a domain structure of Landau–Lifshitz type, *i.e.*, consisting of plate-like domains separated by Bloch walls. This structure can be obtained from the state of homogeneous magnetization of the whole crystal (such as the state of saturation) by rotating the magnetization vector at each lattice site about the same axis, which we assume to be the x_1 -axis. Moreover, if the magnetization vector is assumed to be perpendicular to the x_1 -axis, one can write

$$\vec{\sigma}_f = \sigma_f (0, \cos \varphi_f, \sin \varphi_f), \quad (19)$$

where the rotation angle φ_f depends merely on x_1 .

Then, by multiplying Eq. (18) by n_f^β , where $\beta \neq \alpha$, and subtracting it from the same equation with α and β interchanged, we obtain

$$\begin{aligned} & \frac{1}{8} K [3S^2(S+1)^2 - 6S(S+1) - 5W(\sigma_f)] \sin 2\varphi_f \cos 2\varphi_f + \\ & + \sigma \sum_{g(\neq f)} J_{fg} (\sigma_g^3 \cos \varphi_f - \sigma_g^2 \sin \varphi_f) = 0. \end{aligned} \quad (20)$$

For further calculations we assume $|\varphi_f - \varphi_g| \ll 1$ if f and g are two sites sufficiently near each other along the x_1 -axis. This assumption is reasonably justified by experimental data, as φ can change at most by π on passing through a wall, the wall thickness being at least ten times the lattice constant. Hence, upon passing to continuous variables, $\sigma_f \rightarrow \sigma(x_1)$ ($\varphi_f \rightarrow \varphi(x_1)$), we can use the Taylor series approximation

$$\sigma_g^\alpha = \sigma_f^\alpha + \Delta_{fg} \frac{\partial \sigma_f^\alpha}{\partial x_1} + \frac{1}{2} \Delta_{fg}^2 \frac{\partial^2 \sigma_f^\alpha}{\partial x_1^2}, \quad (21)$$

where

$$\sigma_f^\alpha = \sigma^\alpha(x_1) \Big|_{x_1 \text{ for site } f}, \quad \frac{\partial \sigma_f^\alpha}{\partial x_1} = \frac{\partial \sigma^\alpha(x_1)}{\partial x_1} \Big|_{x_1 \text{ for site } f} \quad (22)$$

and Δ_{fg} is the x_1 -component of the space vector pointing from the lattice site f to the lattice site g .

Substituting (21) to Eq. (20) we obtain

$$\eta \sin 4\varphi + \sigma^2 \gamma \ddot{\varphi} = 0, \quad (23)$$

where

$$\gamma = \frac{1}{2} \sum_{g(\neq f)} J_{fg} \Delta_{fg}^2; \quad \eta = \frac{1}{16} K [3S^2(S+1)^2 - 6S(S+1) - 5W(\sigma)]. \quad (24)$$

By applying to Eqs (17) the same procedure as to Eqs (18) we get

$$\frac{1}{8} K \frac{\partial W \sigma}{\partial \beta M} \left\{ 1 - \frac{5}{4} \sin^2 2\varphi \right\} = \frac{\partial \sigma}{\partial \beta M} \{ M - \tau \sigma + \sigma \gamma \dot{\varphi}^2 \}, \quad (25)$$

where

$$\tau = \sum_{g(\neq f)} J_{fg} \quad (26)$$

and $M = M(x_1)$.

Here, we impose certain symmetry conditions on the crystal lattice which cause terms linear in Δ_{fg} to disappear [3], [12].

In solving Eqs (23) and (25) we use an iteration procedure. In the first step we assume the coefficients in Eq. (23) to be independent of x_1 , and we obtain the first integral

$$\sigma^2 \gamma \dot{\varphi}^2 - \frac{1}{2} \eta \cos 4\varphi = Y \equiv \text{const.} \quad (27)$$

If we restrict ourselves to the so-called asymptotic description of the domain structure (see, e.g., [11], [13]), the constant in Eq. (27) can be determined and Eq. (27) reads

$$\sigma^2 \gamma \dot{\varphi}^2 = \frac{1}{2} \eta \left(\cos 4\varphi + \frac{\eta}{|\eta|} \right). \quad (28)$$

Note that depending on the sign of η the domain centres (*i.e.*, the points at which $\dot{\varphi} = 0$) correspond to

$$\varphi = \pm \frac{\pi}{4}, \pm \frac{3\pi}{4}, \pm \frac{5\pi}{4}, \dots \quad \text{for } \eta > 0$$

and

$$\varphi = 0, \pm \frac{\pi}{2}, \pm \pi, \dots \quad \text{for } \eta < 0. \quad (28a)$$

The use of the simpler asymptotic description of the domain structure is fairly justified, as it was shown in [11], [17] to be a good approximation of the mathematically much more complicated periodic description.

Substituting (28) into (25) we have

$$\frac{1}{8} K\sigma \frac{\partial W(\sigma)}{\partial \beta M} \left\{ 1 - \frac{5}{4} \sin^2 2\varphi \right\} = \frac{\partial \sigma}{\partial \beta M} \left\{ \sigma M - \sigma^2 \tau + \frac{1}{2} \eta \left(\cos 4\varphi + \frac{\eta}{|\eta|} \right) \right\}. \quad (29)$$

Equations (28) and (29) describe the changes in the direction and length of the magnetization vector in the crystal, respectively.

4. Temperature-dependent equation for the domain structure

In order to solve Eq. (29) we use an approximation in calculating the quantities η , $\frac{\partial W(\sigma)}{\partial \beta M}$, $\frac{\partial \sigma}{\partial \beta M}$ which resides in expanding σ into a power series with respect to βM and in assuming this factor to be small, so we can write

$$\sigma = B_s(\beta M) = \frac{K_S^2}{3} \beta M - \frac{K_S^4}{45} (\beta M)^3 + \frac{2K_S^6}{945} (\beta M)^5 - \frac{K_S^8}{4725} (\beta M)^7 + O[(\beta M)^9], \quad (30)$$

where

$$K_S^n = \left(S + \frac{1}{2} \right)^n - \left(\frac{1}{2} \right)^n. \quad (31)$$

One can easily show that

$$\begin{aligned} K_S^4 &= K_S^2 \left(K_S^2 + \frac{1}{2} \right), \\ K_S^6 &= K_S^2 \left\{ \left(K_S^2 \right)^2 + \frac{3}{4} K_S^2 + \frac{3}{16} \right\}, \\ K_S^8 &= K_S^2 \left\{ \left(K_S^2 \right)^3 + \left(K_S^2 \right)^2 + \frac{3}{8} K_S^2 + \frac{1}{16} \right\}. \end{aligned} \quad (32)$$

Then, from (12a), (15), (24) and (30) it follows that

$$\begin{aligned} \eta &= \frac{K}{16} \left[3(K_S^2)^2 - 6K_S^2 - 5 \left\{ (6K_S^2 - 5) \left(\frac{\partial \sigma}{\partial \beta M} + \sigma^2 \right) - 7 \frac{\partial^3 \sigma}{\partial \beta M^3} - 21 \left(\frac{\partial \sigma}{\partial \beta M} \right)^2 - \right. \right. \\ &\quad \left. \left. - 28\sigma \frac{\partial^2 \sigma}{\partial \beta M^2} - 42\sigma^2 \frac{\partial \sigma}{\partial \beta M} - 7\sigma^4 \right\} \right] \\ &= \frac{K}{2 \cdot 3^3 \cdot 5 \cdot 7} K_S^2 (K_S^2 - K_{\frac{1}{2}}^2) (K_S^2 - K_1^2) (K_S^2 - K_{\frac{1}{2}'}^2) (\beta M)^4 + O[(\beta M)^6]. \end{aligned} \quad (33)$$

Here (compare Eq. (31)), $K_{\frac{1}{2}}^2 = \frac{3}{4}$, $K_1^2 = 2$, $K_{\frac{1}{2}'}^2 = \frac{15}{4}$.

Analogically, from (12a), (15) and (30) we obtain

$$\begin{aligned} \sigma \cdot \frac{\partial W(\sigma)}{\partial \beta M} &= [6K_S^2 - 5] \left[\sigma \frac{\partial^2 \sigma}{\partial \beta M^2} + 2\sigma^2 \frac{\partial \sigma}{\partial \beta M} \right] - 7\sigma \frac{\partial^4 \sigma}{\partial \beta M^4} - 70\sigma \frac{\partial \sigma}{\partial \beta M} \frac{\partial^2 \sigma}{\partial \beta M^2} - \\ &- 28\sigma^2 \frac{\partial^3 \sigma}{\partial \beta M^3} - 42\sigma^3 \frac{\partial^2 \sigma}{\partial \beta M^2} - 84\sigma^2 \left(\frac{\partial \sigma}{\partial \beta M} \right)^2 - 28\sigma^4 \frac{\partial \sigma}{\partial \beta M} \\ &= - \frac{2^5}{7 \cdot 5^2 \cdot 3^4} (K_S^2)^2 (K_S^2 - K_{1/2}^2) (K_S^2 - K_1^2) (K_S^2 - K_{1/2}^2) (\beta M)^4 + O[(\beta M)^6]. \end{aligned} \quad (34)$$

Inserting (30), (34) and (33) into (29) we get the following equation

$$\begin{aligned} (\beta M)^2 \left\{ (\beta M)^2 \left[\beta \mathcal{K}_S \left(\frac{3}{10} + \frac{3}{4} \cos 4\varphi + \frac{K}{|K|} \right) + K_S^4 \left(\frac{K_S^2 \tau \beta}{3} - \frac{4}{5} \right) \right] + \right. \\ \left. + 3K_S^2 \left(1 - \frac{K_S^2 \tau \beta}{3} \right) \right\} = 0, \end{aligned} \quad (35)$$

where

$$\mathcal{K}_S = \frac{K}{7 \cdot 5 \cdot 3 \cdot 1} K_S^2 (K_S^2 - K_{1/2}^2) (K_S^2 - K_1^2) (K_S^2 - K_{1/2}^2) = K \prod_{n=0}^3 \frac{(K_S^2 - K_{n/2}^2)}{(2n+1)} \quad (36)$$

and

$$\frac{\eta}{|\eta|} = \frac{K}{|K|}. \quad (37)$$

There are two solutions of Eq. (35) of which the trivial one $\beta M = 0$ is to be rejected as this implies $M = \sigma = 0$ for all T . The second solution is physically meaningful and reads

$$(\beta M)^2 = \frac{3K_S^2 \left(\frac{K_S^2 \tau \beta}{3} - 1 \right)}{\beta \mathcal{K}_S \left(\frac{3}{10} + \frac{3}{4} \cos 4\varphi + \frac{K}{|K|} \right) + K_S^4 \left(\frac{K_S^2 \tau \beta}{3} - \frac{4}{5} \right)}. \quad (38)$$

Taking into account (38), (33) and (30) we easily obtain from (23) the following equation:

$$\begin{aligned} \gamma K_S^2 \left[\beta \mathcal{K}_S \left(\frac{3}{10} + \frac{1}{4} \operatorname{sign} K \right) + \frac{1}{5} K_S^4 (K_S^2 \tau \beta - 2) \right] \ddot{\varphi} + \frac{3}{4} \gamma K_S^2 \mathcal{K}_S \beta \ddot{\varphi} \cos 4\varphi + \\ + \frac{1}{2} (K_S^2 \tau \beta - 3) \mathcal{K}_S \sin 4\varphi = 0. \end{aligned} \quad (39)$$

The first integral of this equation has the form

$$\gamma \dot{\varphi}^2 = \left(\frac{1}{3} \tau - \frac{1}{\beta K_S^2} \right) \ln \left| \beta \mathcal{K}_S \left(\frac{3}{10} + \frac{3}{4} \cos 4\varphi + \frac{1}{4} \operatorname{sign} K \right) + \frac{1}{5} K_S^4 (K_S^2 \tau \beta - 2) \right| + \text{const.} \quad (40)$$

Similarly as in Eq. (27), the constant in Eq. (40) is determined from asymptotic boundary conditions. Thus, if $\eta > 0$ (i.e., $K > 0$) we have $\dot{\varphi} = 0$ for $\varphi = \pm \frac{\pi}{4}, \pm \frac{3\pi}{4}, \dots$ and

$$\text{const} = - \left(\frac{\tau}{3} - \frac{1}{\beta K_S^2} \right) \ln \left| -\frac{1}{5} \beta \mathcal{K}_S + \frac{1}{5} K_S^4 (K_S^2 \beta \tau - 2) \right|; \quad (41)$$

if $\eta < 0$ (i.e., $K < 0$) we have $\dot{\varphi} = 0$ for $\varphi = 0, \pm \frac{\pi}{2}, \pm \pi, \dots$ and

$$\text{const} = - \left(\frac{\tau}{3} - \frac{1}{\beta K_S^2} \right) \ln \left| \frac{4}{5} \beta \mathcal{K}_S + \frac{1}{5} K_S^4 (K_S^2 \beta \tau - 2) \right|. \quad (41a)$$

With the above constants Eq. (40) can be written in the form

$$\gamma \dot{\varphi}^2 = \left(\frac{\tau}{3} - \frac{1}{\beta K_S^2} \right) \ln \left| \frac{\beta \mathcal{K}_S (6 + 5 \text{sign } K + 15 \cos 4\varphi) + 4K_S^4 (K_S^2 \beta \tau - 2)}{2\beta \mathcal{K}_S (3 - 5 \text{sign } K) + 4K_S^4 (K_S^2 \beta \tau - 2)} \right| \quad (42)$$

which holds for $\eta > 0$ as well as for $\eta < 0$. When introducing the quantity

$$T_c = \frac{K_S^2 \tau}{3k}. \quad (43)$$

Eq. (42) can be rewritten as follows:

$$K_S^2 \gamma \dot{\varphi}^2 = k T_c \left(1 - \frac{T}{T_c} \right) \ln \left| \frac{\mathcal{K}_S (6 + 5 \text{sign } K + 15 \cos 4\varphi) + 4k T_c \left[2 \left(1 - \frac{T}{T_c} \right) + 1 \right] K_S^4}{2\mathcal{K}_S (3 - 5 \text{sign } K) + 4K_S^4 k T_c \left[2 \left(1 - \frac{T}{T_c} \right) + 1 \right]} \right|. \quad (44)$$

It is easily proved that the argument of the logarithm is larger than unity. Equation (44) approximately describes the plate-like domain structure with $(90^\circ|90^\circ)$ Bloch walls¹ [13], the temperature being here an independent parameter here. Therefore, we can call Eq. (44) the thermodynamical equation of the domain structure.

5. The temperature dependence of the Bloch wall thickness

The definition of the thickness of the $(90^\circ|90^\circ)$ Bloch wall is (see [13])

$$\delta = \left| \frac{\pi}{2} / \dot{\varphi}_W \right| \quad (45)$$

where $\dot{\varphi}_W$ denotes the value of $\dot{\varphi}$ in the wall centre. By the use of (44) we obtain from (45)

$$\delta = \frac{\pi}{2} \sqrt{\frac{K_S^2 \gamma}{k(T_c - T)}} \ln^{-1/2} \left| \frac{\mathcal{K}_S (3 + 10 \text{sign } K) + 2k T_c \left[2 \left(1 - \frac{T}{T_c} \right) + 1 \right] K_S^4}{\mathcal{K}_S (3 - 5 \text{sign } K) + 2k T_c \left[2 \left(1 - \frac{T}{T_c} \right) + 1 \right] K_S^4} \right|. \quad (46)$$

¹ According to [9] the symbol for a Bloch wall is (Ψ, Φ) , where Ψ denotes the angle between the magnetization vectors of two neighbouring domains, and Φ is the angle by which the magnetization vectors rotates on passing through the wall.

In estimating the influence of the temperature on the wall thickness the above formula can be simplified somewhat. First note that the argument of the logarithm in Eq. (46) can be written in the form $1+A$ where $A > 0$. A rough estimation easily shows that $10^{-5} < A < 10^{-2}$. Hence, we have for the thickness δ the approximate formula

$$\delta \approx \frac{\pi}{2} \sqrt{\frac{4\gamma K_S^3 K_S^4}{15|\chi_S|} + \frac{T_c}{T_c - T} \left\{ \frac{\gamma}{\tau} \left(\frac{3}{5} \text{sign } K - 1 \right) + \frac{2\gamma K_S^3 K_S^4}{15|\chi_S|} \right\}}. \tag{47}$$

Another very simple and convenient formula can be obtained when noting that the temperature T does not strongly influence the value of the logarithm in Eq. (46). Therefore, we can write for two arbitrary temperatures, T_1 and T_2

$$\frac{\delta_{T_1}}{\delta_{T_2}} \approx \sqrt{\frac{T_c - T_2}{T_c - T_1}} \tag{48}$$

the approximation in Eq. (48) being the better the smaller the difference between T_1 and T_2 . The relation (48) is presented in Fig. 1 for a fixed temperature T_2 . We shall illustrate the temperature dependence of the Bloch wall thickness on some quantitative results for Fe.

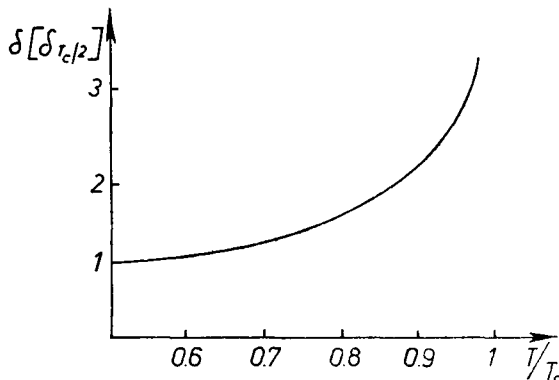


Fig. 1. Dependence of relative wall thickness on reduced temperature

In this case we have $T_c = 1043^\circ\text{K}$. Furthermore, we shall take into account the change of the lattice constant a with temperature [14]. By comparing our free energy (16) with its phenomenological counterpart, e.g., in [15], one can easily establish the relationship between our microscopic anisotropy constant K and the macroscopic anisotropy constant K_1 . From (16) and (24) we have

$$|K_1| = 2|\eta|. \tag{49}$$

Taking into account Eq. (12a) we obtain for $T = 0$

$$|K_1| = \left| K \prod_{n=0}^3 \left(S - \frac{n}{2} \right) \right|. \tag{50}$$

With $K_1 = 5.8 \times 10^5 \text{ erg/cm}^3$ for Fe (for $T=0$ [16]) we obtain ((47), (50)) for the $(90^\circ|90^\circ)$ Bloch wall thickness in iron the values presented in Table I and Fig. 2. The Bloch wall thicknesses estimated experimentally at room temperature are of the same order of magnitude as those given in Table I.

TABLE I

$T^\circ\text{K}$	$s = 1/2$		$s = 1$		$s = 2$		$s = \infty$	
	$\delta [\text{\AA}]$	$\delta [a]$	$\delta [\text{\AA}]$	$\delta [a]$	$\delta [\text{\AA}]$	$\delta [a]$	$\delta [\text{\AA}]$	$\delta [a]$
0	527	185	798	279	1174	411	2584	906
273	558	195	845	295	1243	434	2746	956
473	594	207	899	313	1323	461	2914	1015
673	667	232	1009	351	1485	516	3269	1136
873	868	301	1314	456	1933	670	4255	1475
973	1250	433	1892	655	2784	964	6129	2123

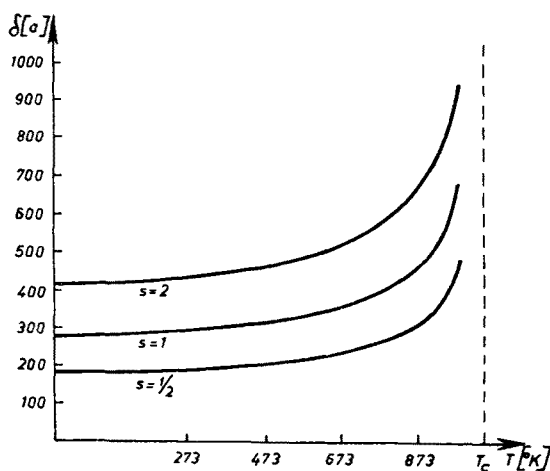


Fig. 2. Dependence of wall thickness on temperature for Fe, for three spin values; $s = 1/2, 1, 2$. (a — lattice constant)

6. Final remarks

The main result of our paper is the derivation of the temperature dependence of the Bloch wall thickness, Eqs (46), (47) and (48), which is illustrated by evaluations for Fe, Eq. (49) and Table I. These results were obtained by means of an iteration procedure. In the first step the coefficients in Eq. (23) are assumed to be constant in the whole crystal (σ independent of φ). In this way, and by using a high-temperature expansion for the Brillouin function, the formula (38) for βM was derived. It is to be noted that in this approximation βM is equal to zero when

$$\frac{K_1^2 \tau \beta}{3} - 1 = 0, \quad (51)$$

(see Eq. (38)) or, equivalently,

$$T = \frac{K_S^2 \tau}{3k} \equiv T_0$$

which coincides with the definition of T_c (Eq. (43)). As according to Eq. (9), σ vanishes for $T = T_0$, the latter is to be identified with the Curie temperature in the present approximation. In the next step, βM given by formula (38) was inserted into Eq. (23) and we obtained a temperature-dependent equation for the domain structure which, in turn, was the basis for the calculations in Sec. 5.

APPENDIX I

In order to calculate $\langle A \rangle_0$ which is defined in Eq. (11) we take into account the form of tensor $Q_{fg}^{\alpha\beta\gamma\delta}$ according to (3) and we have

$$\langle A \rangle_0 = \frac{1}{2} K \left\langle \sum_{f,g} \sum_{\alpha,\beta,\gamma,\delta} \delta_{fg} \delta^{\alpha\beta} \delta^{\gamma\delta} (1 - \delta^{\alpha\delta}) S_f^\alpha S_f^\beta S_g^\gamma S_g^\delta \right\rangle_0 \quad (\text{A})$$

Then, we have

$$\langle A \rangle_0 = \frac{1}{2} K \left\langle \sum_f \sum_{\alpha \neq \delta} S_f^\alpha S_f^\alpha S_f^\delta S_f^\delta \right\rangle_0 \quad (\text{B})$$

Let us pass to local coordinate systems

$$S_f^\alpha = \sum_\tau a_{\alpha\tau} S_f^\tau \quad (\text{C})$$

We introduce new local coordinate systems (the primes) by taking the x'_3 axes parallel to the vectors of the molecular field \vec{M}_f in each site f ; therefore, the direction of this axis can change from site to site. Strictly speaking, the indices of the matrix transformation to the local coordinate system should have an additional index of the site. We will omit it, however, in order to simplify the notation. With (C) we have

$$(S_f^\alpha)^2 = (a_{\alpha 1} S_f'^1)^2 + (a_{\alpha 2} S_f'^2)^2 + (a_{\alpha 3} S_f'^3)^2 + \\ + a_{\alpha 1} a_{\alpha 2} (S_f'^1 S_f'^2 + S_f'^2 S_f'^1) + a_{\alpha 1} a_{\alpha 3} (S_f'^1 S_f'^3 + S_f'^3 S_f'^1) + a_{\alpha 2} a_{\alpha 3} (S_f'^2 S_f'^3 + S_f'^3 S_f'^2). \quad (\text{D})$$

Let us go over at present in local coordinate system from the operators S_f^α to $S_f'^+$, $S_f'^-$, $S_f'^3$ according to the relations

$$S_f'^1 = \frac{1}{2} (S_f'^+ + S_f'^-), \quad S_f'^2 = \frac{1}{2} (S_f'^- - S_f'^+), \quad S_f'^3 = S_f'^3. \quad (\text{E})$$

By performing some algebraic calculations we get

$$(S_f^\alpha)^2 = \frac{1}{4} a_{\alpha 1}^2 [S_f'^- S_f'^- + S_f'^+ S_f'^+ + 2S(S+1) - 2(S_f'^3)^2] - \frac{1}{4} a_{\alpha 2}^2 [S_f'^- S_f'^- +$$

$$\begin{aligned}
& + S_f' + S_f'^+ - 2S(S+1) + 2(S_f'^3)^2 + a_{\alpha 3}^2 (S_f'^3)^2 + \frac{i}{2} a_{\alpha 1} a_{\alpha 2} (S_f'^- S_f'^- - S_f'^+ S_f'^+) + \\
& + \frac{1}{2} a_{\alpha 1} a_{\alpha 3} (S_f'^- S_f'^3 + S_f'^+ S_f'^3 + S_f'^3 S_f'^- + S_f'^3 S_f'^+) + \frac{i}{2} a_{\alpha 2} a_{\alpha 3} (S_f'^- S_f'^3 - \\
& - S_f'^+ S_f'^3 + S_f'^3 S_f'^- - S_f'^3 S_f'^+); \tag{F}
\end{aligned}$$

where account is taken of the relations

$$\begin{aligned}
S_f'^- S_f'^+ &= S(S+1) - S_f'^3 - S_f'^3 S_f'^3 \\
S_f'^+ S_f'^- &= S(S+1) + S_f'^3 - S_f'^3 S_f'^3. \tag{G}
\end{aligned}$$

With (F) we can obtain, for example,

$$\begin{aligned}
(S_f'^1 S_f'^2 S_f'^3 + S_f'^2 S_f'^1 S_f'^3) &= [S_f'^- S_f'^- S_f'^+ S_f'^+ + S_f'^+ S_f'^+ S_f'^- S_f'^-] \left[\frac{1}{8} a_{11}^2 a_{21}^2 - \frac{1}{8} a_{11}^2 a_{22}^2 - \right. \\
& - \frac{1}{8} a_{21}^2 a_{12}^2 + \frac{1}{8} a_{12}^2 a_{22}^2 + \frac{1}{2} a_{11} a_{12} a_{21} a_{22} \left. \right] + \frac{1}{2} S^2 (S+1)^2 [a_{11}^2 a_{21}^2 + a_{11}^2 a_{22}^2 + a_{21}^2 a_{12}^2 + \\
& a_{12}^2 a_{22}^2] + S(S+1) S_f'^3 S_f'^3 [-a_{11}^2 a_{21}^2 - a_{11}^2 a_{22}^2 - a_{21}^2 a_{12}^2 - a_{12}^2 a_{22}^2 + a_{21}^2 a_{13}^2 + a_{22}^2 a_{13}^2 + a_{23}^2 a_{12}^2 + a_{11}^2 a_{23}^2] + \\
& + S_f'^3 S_f'^3 S_f'^3 S_f'^3 \left[\frac{1}{2} a_{11}^2 a_{21}^2 + \frac{1}{2} a_{11}^2 a_{22}^2 + \frac{1}{2} a_{21}^2 a_{12}^2 + \frac{1}{2} a_{12}^2 a_{22}^2 - a_{21}^2 a_{13}^2 - a_{22}^2 a_{13}^2 - a_{23}^2 a_{12}^2 - \right. \\
& - a_{11}^2 a_{23}^2 + 2a_{13}^2 a_{23}^2 \left. \right] + \frac{1}{2} [S_f'^- S_f'^3 S_f'^+ S_f'^3 + S_f'^- S_f'^3 S_f'^3 S_f'^+ + S_f'^3 S_f'^- S_f'^+ S_f'^3 + S_f'^+ S_f'^3 S_f'^- S_f'^3 + \\
& + S_f'^3 S_f'^- S_f'^3 S_f'^+ + S_f'^3 S_f'^- S_f'^- S_f'^3 + S_f'^+ S_f'^3 S_f'^3 S_f'^- + \\
& + S_f'^3 S_f'^+ S_f'^3 S_f'^-] [a_{11} a_{13} a_{21} a_{23} + a_{13} a_{12} a_{22} a_{23}] \equiv g(a_{1x}, a_{2y}; S_f'^+, S_f'^-, S_f'^3). \tag{H}
\end{aligned}$$

It is easily shown that

$$\begin{aligned}
[S_f'^1 S_f'^1, S_f'^2 S_f'^2]_{\pm} &= g(a_{1x}, a_{2y}; S_f'^+, S_f'^-, S_f'^3) \\
[S_f'^1 S_f'^1, S_f'^3 S_f'^3]_{\pm} &= g(a_{1x}, a_{3y}; S_f'^+, S_f'^-, S_f'^3) \\
[S_f'^2 S_f'^2, S_f'^3 S_f'^3]_{\pm} &= g(a_{2x}, a_{3y}; S_f'^+, S_f'^-, S_f'^3) \tag{J}
\end{aligned}$$

With (B), (H) and (J) we have

$$\begin{aligned}
\langle A \rangle_0 &= \frac{1}{2} K \left\langle \sum_f [g(a_{1x}, a_{2y}; S_f'^+, S_f'^-, S_f'^3) + g(a_{1x}, a_{3y}; S_f'^+, S_f'^-, S_f'^3) + \right. \\
& \left. + g(a_{2x}, a_{3y}; S_f'^+, S_f'^-, S_f'^3)] \right\rangle_0. \tag{K}
\end{aligned}$$

Introducing the direction cosines with respect to the x'_3 axis as follows

$$n_f^1 = a_{13}, \quad n_f^2 = a_{23}, \quad n_f^3 = a_{33} \tag{L}$$

and taking into consideration the relations

$$\sum_{k=1}^3 a_{ik} a_{jk} = \delta_{ij} \quad (M)$$

we obtain with (K), (J) and (H) the following equation:

$$\langle A \rangle_0 = \frac{1}{2} K \left\langle \sum_f \left\{ \frac{1}{8} [S_f' - S_f'^-, S_f' + S_f'^+] + (N_f - 1) + \frac{1}{2} S^2(S+1)^2(N_f+1) + S(S+1)S_f'^3 S_f'^3 (1-3N_f) + \frac{3}{2} S_f'^3 S_f'^3 S_f'^3 S_f'^3 (3N_f-1) - \frac{1}{2} N_f [[S_f'^3 S_f'^-]_+, [S_f'^3 S_f'^+]_{+1}] \right\} \right\rangle_0 \quad (N)$$

where

$$N_f = (n_f^1)^2 (n_f^2)^2 + (n_f^2)^2 (n_f^3)^2 + (n_f^3)^2 (n_f^1)^2. \quad (P)$$

Taking into account the following commutation relations

$$[S_f'^+, S_f'^-]_- = 2S_f'^3, \quad [S_f'^\pm, S_f'^3]_- = \mp S_f'^\pm \quad (R)$$

and (G), we finally obtain

$$\langle A \rangle_0 = \frac{1}{8} K \sum_f \left\{ 2S(S+1) + S^2(S+1)^2 + [6S(S+1) - 5] \langle (S_f'^3)^2 \rangle_0 - 7 \langle (S_f'^3)^4 \rangle_0 - \frac{1}{2} \sum_{\alpha \neq \beta} (n_f^\alpha)^2 (n_f^\beta)^2 \left[6S(S+1) - 3S^2(S+1)^2 + 5[6S(S+1) - 5] \langle (S_f'^3)^2 \rangle_0 - 35 \langle (S_f'^3)^4 \rangle_0 \right] \right\}. \quad (S)$$

The above equation coincides with (12) and (12a).

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