ENERGIES OF 90°, 71° AND 109° BLOCH WALL CLASSES IN CUBIC FERROMAGNETIC LATTICES

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On the basis of a uniform method developed by Ziętek the relative energies for all possible orientations of 90°, 71° and 109° Bloch walls in cubic ferromagnetic lattices are numerically calculated and the corresponding curves given. The dependence of the energies on the crystallographic orientation is used to examine the stability of certain domain structures. The results obtained are complementary to those derived by other authors.

1. Introduction

Ferromagnetic crystals characterize by the existence of a domain structure, *i. e.*, the crystal is divided into domains magnetized in different crystallographic directions (directions of easiest magnetization). In the body centred cubic lattice (*e.g.*, Fe), there are six such directions which coincide with the crystallographic axes of type ⟨100⟩; in the face centred cubic lattice (*e. g.*, Ni), one has eight those directions that correspond to the crystallographic axes ⟨111⟩ (see Figs 1 and 2).

The boundary between two neighbouring domains is, generally speaking, the region in which the magnetization changes its position from one easy direction to another. When within the domain boundary the magnetization changes its position by rotating around an axis which is perpendicular to the boundary, the latter is called a Bloch wall. In bulk crystals Bloch walls are energetically more favourable than those with the rotation axis parallel to the plane of the boundary (Néel walls), as in the latter case free magnetic poles are produced within the wall which increases the energy considerably.

It is easily seen that for two arbitrary easy directions shown in Fig. 1 or 2 there is, from the geometrical point of view, an infinite number of Bloch walls with different crystallo-

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graphical orientation by which the transition between these easy directions can be realized. Let us denote by $\boldsymbol{a}$ and $\boldsymbol{b}$ the unit vectors which indicate any two easy directions in the crystal, and by $\boldsymbol{e}$ the unit vector which defines the rotation axis of the Bloch wall. Then, two cases are to be considered:

i) $\boldsymbol{a} = -\boldsymbol{b}$. The magnetization vectors of adjacent domains form an angle of 180° and, according to Figs 1 and 2, this case takes place in the bcc as well as in the fcc lattice. The condition for such a 180°. Bloch wall class is $\boldsymbol{e} \cdot \boldsymbol{a} = 0$.

ii) $\boldsymbol{a} \neq -\boldsymbol{b}$. In the bcc lattice, the magnetization vectors of adjacent domains form then, according to Fig. 1, an angle of 90°, and in the fcc lattice, according to Fig. 2, the

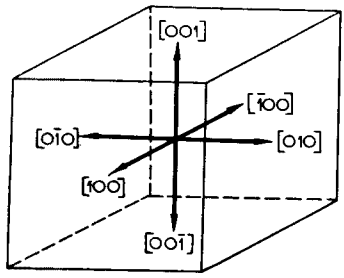

Fig. 1. Directions of easiest magnetization in the bcc lattice

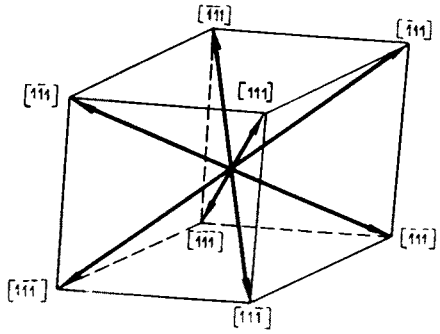

Fig. 2. Directions of easiest magnetization in the fcc lattice

angles $\sim 71°$ or $\sim 109°$ (the angle 71° is formed, for example, by the directions [1$\bar{1}$1] and [1$\bar{1}\bar{1}$], and the angle 109° by the directions [1$\bar{1}$1] and [$\bar{1}$11]). The condition for the respective (*i. e.*, 90°, 71° and 109°) Bloch wall classes is in this case $\boldsymbol{e}(\boldsymbol{a}-\boldsymbol{b}) = 0$. Consequently, the rotation of the magnetization vector in the Bloch wall takes now place on a cone and the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ will, in general, lie asymmetrically on it; this results in two different rotation angles (left- and right-hand rotation) by which one can pass from $\boldsymbol{a}$ to $\boldsymbol{b}$. Denoting by Φ the smaller of those angles we note the relation

$$\gamma \leqslant \Phi \leqslant \pi$$

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where γ stands for 90°, 71° or 109°, respectively. Therefore, in the case of 90°, 71° or 109° Bloch wall classes the crystallographic orientation (*i. e.*, the vector $\boldsymbol{e}$) does not determine completely a Bloch wall because there are still two possibilities, namely, the rotations Φ or $2\pi-\Phi$ by which it can be realized. For few particular orientations of the rotation axis it happens that beside the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ also some other easy directions are lying on the cone. In that case, two or three Bloch walls may be produced when passing from $\boldsymbol{a}$ to $\boldsymbol{b}$.

The Bloch wall energies for the respective classes were already calculated in some papers [1], [2], [3] (*cf.* [4] pp. 286—290). The problem investigated in the present paper is the same, the differences residing in the approach.

In the papers [1], [2], [3] the energy density of a single Bloch wall as a function of its crystallographic orientation was calculated on the basis of a formula derived first by Néel [5]. However, the considerations of the 90°, 71° and 109° Bloch walls were restricted to the angle Φ. It is easily seen that a periodic domain structure constructed of that type of Bloch walls would necessarily lead to the same polarization of all Bloch walls, as the rotation angle φ of the magnetization vector on passing through each wall is restricted to the interval $[0, \Phi]$. Thus, the rotation in successive walls alternates from a left-hand (φ increases from 0 to Φ) to a right-hand one (φ decreases from Φ to 0).

It is well known from experiment that in typical ferromagnetic domain structures the rotation of the magnetization vector occures in the same sense on passing from domain to domain, being either left-handed or right-handed throughout the crystal (or at least over large regions containing many domains, see [6, 7]). As a result, the polarization of successive Bloch walls is not the same, *e. g.*, successive 180° Bloch walls have opposite polarizations. It is obvious that lattice sites of which the magnetization vectors have the same direction correspond to rotation angles $\varphi+2n\pi$, $n = 0, \pm1, \pm2, \ldots$ Therefore, for a given rotation axis the energies of Bloch walls generated by the rotation on Φ as well as on $2\pi-\Phi$ should be taken into account, which is equivalent to considering the energy of a rotation over 2π.

We shall examine only the 90°, 71° and 109° Bloch wall classes. The 180° case is trivial (for the bcc as well as for the fcc lattice) because the energies for the left-hand and right-hand rotation are identical[1] ($\Phi = \pi$ for the whole class).

Our calculations are based on a uniform method developed by Ziętek [8], which, in the simplest approximation we use, corresponds to the phenomenological approach [9]. We take into account only the isotropic exchange energy and the anisotropic magnetocrystalline energy. Others factors, *i. e.*, magnetostriction as well as surface phenomena are omitted.

Finally, it has to be pointed out that in evaluating the integrals we use the asymptotic description of Bloch walls [9] instead of the periodic one [10], which for domain widths of the order 10^{-2} cm leads to an error of less than 1% in calculating Bloch wall energies [11].

The integrals in our paper were evaluated numerically by Simpson's Rule using an electronic computer.

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[1] As for the 90° case, the energy for the rotation on $2\pi-\Phi$ was also calculated by Graham [2], so the energy corresponding to 2π can be obtained from this paper by simply summing the energies for Φ and $2\pi-\Phi$. However, for two reasons we decide to repeat those calculations. Firstly, the integrals in [2] were evaluated graphically and, secondly, this evaluation was done for few domain wall orientations only.

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2. General assumptions

Following [8] we start with the formula for the average energy, h, of the crystal

$$h = S^2 \sum_{\alpha\beta} \{\tilde{P}^{\alpha\beta}_{33} + \tilde{Q}^{\alpha\beta}\}, \tag{1}$$

where

$$\tilde{P}^{\alpha\beta}_{33} = A^{\alpha\beta} R^{\alpha}_{\mu 3} R^{\beta}_{\mu 3}, \tag{2}$$

$$\tilde{Q}^{\alpha\beta} = K\delta^{\alpha\beta}\left\{\frac{1}{4} + S + \left(S - \frac{1}{2}\right)^2 [(R^{\alpha}_{13})^2 - (R^{\alpha}_{13})^4 + (R^{\alpha}_{23})^2 (R^{\alpha}_{33})^2]\right\}, \tag{3}$$

$$R^{\alpha}_{\mu\nu} = \varepsilon_{\mu\sigma\nu} e_{\sigma} \sin\varphi^{\alpha} + \delta_{\mu\nu} \cos\varphi^{\alpha} + e_{\mu} e_{\nu}(1 - \cos\varphi^{\alpha}). \tag{4}$$

The particular forms (2) and (3) of $\tilde{P}^{\alpha\beta}_{33}$ and $\tilde{Q}^{\alpha\beta}$ were derived in [12], [13], where in the spin operator Hamiltonian

$$H = \sum_{\alpha\beta} \{P^{\alpha\beta}_{\mu_1\mu_2} S^{\alpha}_{\mu_1} S^{\beta}_{\mu_2} + Q^{\alpha\beta}_{\mu_1\mu_2\mu_3\mu_4} S^{\alpha}_{\mu_1} S^{\alpha}_{\mu_2} S^{\beta}_{\mu_3} S^{\beta}_{\mu_4}\} \tag{5}$$

the interaction tensors were chosen in the form

$$P^{\alpha\beta}_{\mu_2\mu_1} = A^{\alpha\beta}\delta_{\mu_1\mu_2}(1 - \delta^{\alpha\beta}), \tag{6}$$

$$Q^{\alpha\beta}_{\mu_1\mu_2\mu_3\mu_4} = \frac{1}{2} K\delta^{\alpha\beta}\delta_{\mu_1\mu_2}\delta_{\mu_3\mu_4}(1 - \delta_{\mu_1\mu_4}), \tag{7}$$

the latter being matched in correspondence to the classical phenomenological anisotropy energy [12, 10]. Here and in the following, only the lower indices obey the Einstein summation convention. The superscript α, β refer to the lattice sites, β denoting neighbours of the site α. The matrix $R^{\alpha}_{\mu\nu}$ rotates the spin vector S^{α}_{ν} by an angle φ^{α} around an axis with direction cosines e_{μ}. $\varepsilon_{\mu\sigma\nu}$ is the antisymmetric unit pseudotensor, $A^{\alpha\beta}$ stands for the isotropic Heisenberg exchange integral, and K is the "microscopic" anisotropy constant (per atom; see [10]). It has to be noted that Eq. (1) was derived under the assumption that the component S_3 of the spin vector be diagonal, with S as the maximum spin eigenvalue.

As we shall take into consideration the interactions with the nearest neighbours only, we can put in (2) $A^{\alpha\beta} = A$.

The matrix $R^{\alpha}_{\mu\nu}$ is quite general *i. e.*, it describes an arbitrary rotation, and two of the three direction cosines e_{μ} are independent parameters. In our further calculations the rotation axis will be assumed to lie on a fixed plane, which reduces the number of independent parameters e_{μ} to one that describes the position of the rotation axis in the plane.

3. The 90° Bloch wall class in the bcc lattice

We considere a periodic domain structure in which the direction of the magnetization vectors in adjacent domains differs by an angle 90°. This structure can be obtained by putting $\boldsymbol{a} \,||\, [001]$ and $\boldsymbol{b} \,||\, [100]$. By choosing the coordinate system as shown in Fig. 3 we

have for the direction cosines e_μ

$$e_1 = e_3 = \frac{1}{\sqrt{2}} \cos\psi, \qquad e_2 = \sin\psi. \tag{8}$$

Here ψ is an angle between the rotation axis and the (010) plane.

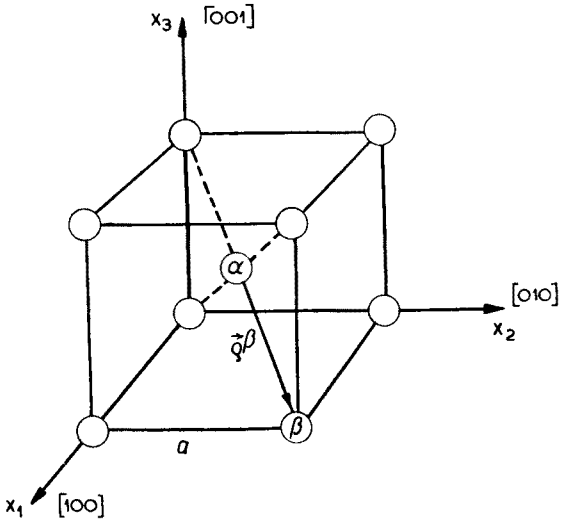

Fig. 3. Elementary cube of the bcc lattice ($\beta = 1, 2, \ldots 8$)

Hence, the elements $R^\alpha_{\mu 3}$ of the rotation matrix have the form

$$R^\alpha_{13} = \sin\psi \sin\varphi^\alpha + \frac{1}{2}\cos^2\psi(1-\cos\varphi^\alpha),$$

$$R^\alpha_{23} = -\frac{1}{\sqrt{2}}\cos\psi \sin\varphi^\alpha + \frac{1}{\sqrt{2}}\cos\psi \sin\psi\,(1-\cos\varphi^\alpha),$$

$$R^\alpha_{33} = \cos\varphi^\alpha + \frac{1}{2}\cos^2\psi\,(1-\cos\psi^\alpha). \tag{9}$$

From (2) it then follows

$$\sum_{\beta=1}^{8} \tilde{P}^{\alpha\beta}_{33} = A\left[4\cos^2\psi + \left(1-\frac{1}{2}\cos^2\psi\right)\sum_{\beta=1}^{8}\cos(\varphi^\beta-\varphi^\alpha)\right]. \tag{10}$$

Following the usual procedure [8, 12] we shall now express φ^β in terms of φ^α and its first derivative. We assume the angle φ^α (or φ^β) to be identical for all lattice atoms lying in the same plane perpendicular to the rotation axis. For a given rotation axis, the problem becomes one-dimensional and, in the first approximation of a Taylor series, we have

$$\varphi^\beta = \varphi^\alpha + e_\mu \varrho^\beta_\mu \dot{\varphi}^\alpha \tag{11}$$

where the dot above φ^α denotes differentiation with respect to a variable ξ taken along the rotation axis, and ϱ_μ^β the components of the space vector pointing from any atom α to its nearest neighbour β. Then, expanding $\cos(e_\mu \varrho_\mu^\beta \dot{\varphi}^\alpha)$ in a series with respect to $e_\mu \varrho_\mu^\beta \dot{\varphi}^\alpha$ we get in the second order approximation

$$S^2 \sum_\beta \tilde{P}_{33}^{\alpha\beta} = 8\,AS^2 - \left(\frac{1}{2} - \frac{1}{4}\cos^2\psi\right) S^2 A\,(\dot{\varphi}^\alpha)^2 \sum_\beta (e_\mu \varrho_\mu^\beta)^2$$

$$= 8\,AS^2 - \left(1 - \frac{1}{2}\cos^2\psi\right) S^2 A a^2\,(\dot{\varphi}^\alpha)^2. \tag{12}$$

In the last step we made use of Eq. (I.4) derived in Appendix I. Denoting

$$\left(\frac{1}{2}\cos^2\psi - 1\right) S^2 A a^2 = U_0 \tag{13}$$

the Eq. (12) can be rewritten as

$$S^2 \sum_\beta \tilde{P}_{33}^{\alpha\beta} = 8AS^2 + U_0(\dot{\varphi}^\alpha)^2. \tag{14}$$

By using Eqs. (3) and (9) we obtain

$$S^2\,\tilde{Q}^{\alpha\beta} = C - V_1 \sin\varphi^\alpha - V_2 \sin 2\varphi^\alpha - V_3 \sin 3\varphi^\alpha - V_4 \sin 4\varphi^\alpha -$$

$$- U_1 \cos\varphi^\alpha - U_2 \cos 2\varphi^\alpha - U_3 \cos 3\varphi^\alpha - U_4 \cos 4\varphi^\alpha, \tag{15}$$

the coefficients $V_1 \ldots U_4$ are given in Appendix II and C is a constant (depending on ψ) which is of no importance in our further calculations and need not be specified here.

According to Eq. (III. 8) derived in Appendix III the energy per cm^2 of the 90° Bloch walls is given by the expression

$$\sigma = \sigma_0 \sqrt{4 - 2\cos^2\psi} \int_0^{2\pi} [-v_1 \sin\varphi - v_2 \sin 2\varphi - v_3 \sin 3\varphi -$$

$$- v_4 \sin 4\varphi - u_1 \cos\varphi - u_2 \cos 2\varphi - u_3 \cos 3\varphi - u_4 \cos 4\varphi + u_1 + u_2 + u_3 + u_4]^{1/2} d\varphi, \tag{16}$$

where

$$\sigma_0 = 2S^2 \left(S - \frac{1}{2}\right) a^{-2} \sqrt{-AK}, \tag{17}$$

and

$$v_i = V_i / KS^2 \left(S - \frac{1}{2}\right)^2, \quad u_i = U_i / KS \left(S - \frac{1}{2}\right)^2,$$

$$(i = 1, 2, 3, 4). \tag{18}$$

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The integral in Eq. (16) was calculated numerically for ψ changing by 1° from 0° to 90° The results are given by the curve σ/σ_0 (relative energy) in Fig. 4.

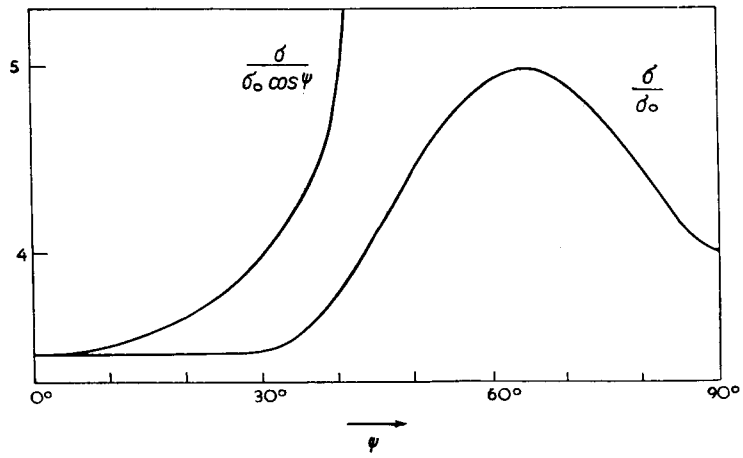

Fig. 4. Relative 90° Bloch walls energy per unit area σ/σ_0 and total Bloch walls energy $\sigma/\sigma_0 \cos\psi$ *vs* Bloch walls orientation ψ

4. The 71° and 109° Bloch wall classes in the fcc lattice

To generate these classes of walls one should start from a direction of the type $\langle 111\rangle$ and, as formula (1) has been derived under the assumption that the initial direction of quantization of the spin operators coincides with the x_3-axis, a coordinate system in which the x_3-axis coincides with, say, the $[1\bar{1}1]$ direction has to be chosen. However, the form of the anisotropy tensor $Q^{\alpha\beta}_{\mu_1\mu_2\mu_3\mu_4}$ in (7) corresponds to a coordinate system whose axes coincide with the [100], [010], and [001] crystallographic directions.

This difficulty can be overcome and the coordinate system indicated in Fig. 5 still used when, as shown in [12], the uniform rotation

$$(V_{\mu\nu}) = \frac{\sqrt{3}}{6}\begin{pmatrix} \sqrt{3}+1 & \sqrt{3}-1 & 2 \\ \sqrt{3}-1 & \sqrt{3}+1 & -2 \\ -2 & 2 & 2 \end{pmatrix} \tag{19}$$

by which all the spins are rotated towards the crystallographic direction $[1\bar{1}1]$ is performed before applying the non-uniform transformation (4).

The total transformation $W^{\alpha}_{\mu\nu}$ is thus

$$W^{\alpha}_{\mu\nu} = R^{\alpha}_{\mu\lambda} V_{\lambda\nu}, \tag{20}$$

and, in order to calculate the quantities $\tilde{P}^{\alpha\beta}_{33}$ and $\tilde{Q}^{\alpha\beta}$ in Eq. (1), one has now to exchange $R^{\alpha}_{\mu 3}$ for $W^{\alpha}_{\mu 3}$ in Eqs. (2) and (3).

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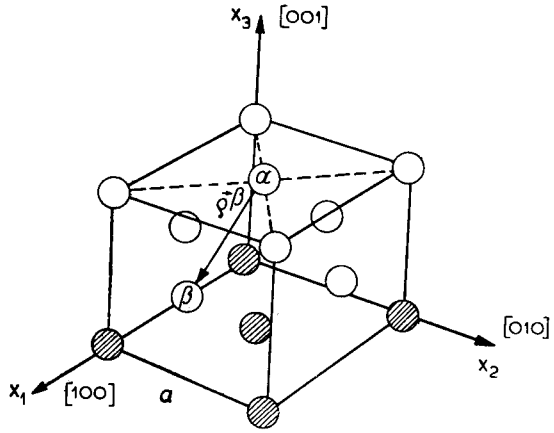

Fig. 5. Elementary cube of the fcc lattice ($\beta = 1, 2, \ldots, 12$). White circles indicate the nearest neighbours

4.1. The 71° Bloch wall class

When starting from the direction $[1\bar{1}1]$ one has $\boldsymbol{a} \parallel [1\bar{1}1]$ and, say, $\boldsymbol{b} \parallel [1\bar{1}\bar{1}]$. For the coordinate system shown in Fig. 5 we have for the direction cosines e_μ

$$e_1 = \frac{1}{\sqrt{2}}(\cos\psi + \sin\psi),\ e_2 = \frac{1}{\sqrt{2}}(\sin\psi - \cos\psi),$$
$$e_3 = 0, \tag{21}$$

where ψ is the angle between the rotation axis and the direction $[1\bar{1}0]$.

By use of Eqs (4), (19), (20) and (21) we have

$$W^\alpha_{13} = \frac{1}{\sqrt{3}}[\cos^2\psi + \cos\psi\sin\psi + (\sin^2\psi - \sin\psi\cos\psi)\cos\varphi^\alpha + \frac{1}{\sqrt{2}}(\sin\psi - \cos\psi)\sin\varphi^\alpha],$$

$$W^\alpha_{23} = \frac{1}{\sqrt{3}}[-\cos^2\psi + \sin\psi\cos\psi - (\sin^2\psi + \sin\psi\cos\psi)\cos\varphi^\alpha - \frac{1}{\sqrt{2}}(\sin\psi + \cos\psi)\sin\varphi^\alpha],$$

$$W^\alpha_{33} = \frac{1}{\sqrt{3}}[-\sqrt{2}\sin\psi\sin\varphi^\alpha + \cos\varphi^\alpha]. \tag{22}$$

From (2) and (22) we have

$$\sum_\beta \tilde{P}^{\alpha\beta}_{33} = A\left[4 + 4\cos 2\psi + \frac{1}{3}(2 - \cos 2\psi)\sum_\beta \cos(\varphi^\beta - \varphi^\alpha)\right] \tag{23}$$

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and, following the procedure of Sec. 3, we finally obtain

$$S^2 \sum_{\beta} \tilde{P}_{33}^{\alpha\beta} = 12AS^2 + U^2(\dot{\varphi}^{\alpha})^2, \tag{24}$$

where

$$U_0 = \frac{1}{3}(\cos 2\psi - 2) AS^2 a^2. \tag{25}$$

Inserting (22) in (3) one gets for $S^2 \tilde{Q}^{\alpha\beta}$ the formula identical with that given by Eq. (15) with the coefficients $V_1 \ldots U_4$ defined in Appendix IV and a constant C (depending on ψ) which need not be specified here.

Using Eq. (III. 8) we have for the energy of the 71° Bloch walls.

$$\sigma = \sigma_0 \sqrt{\frac{4}{3}(2-\cos 2\psi)} \int_0^{2\pi} [+v_1 \sin\varphi + v_2 \sin 2\varphi + v_3 \sin 3\varphi +$$

$$+ v_4 \sin 4\varphi + u_1 \cos\varphi + u_2 \cos 2\varphi + u_3 \cos 3\varphi + u_4 \cos 4\varphi - u_1 - u_2 - u_3 - u_4]^{1/2} d\varphi \tag{26}$$

where

$$\sigma_0 = 4S^2 \left(S - \frac{1}{2}\right) a^2 \sqrt{AK}. \tag{27}$$

For v_i and u_i Eqs (18) still hold, with $V_1 \ldots U_4$ from Appendix IV.

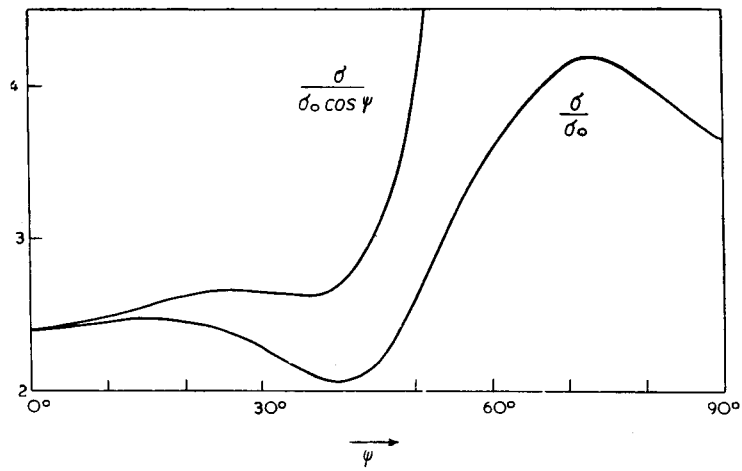

Fig. 6. Relative 71° Bloch walls energy per unit area σ/σ_0 and total Bloch walls energy $\sigma/\sigma_0 \cos\psi$ *vs* Bloch walls orientation ψ

The integral in Eq. (26) was calculated numerically for ψ changing by 1° from 0° to 90°. The results are given by the curve σ/σ_0 in Fig. 6.

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4.2. The 109° Bloch wall class

For this class we have $\boldsymbol{a} \parallel [1\bar{1}1]$ and $\boldsymbol{b} \parallel [\bar{1}11]$. The direction cosines of the rotation axis are now

$$e_1 = e_2 = -\frac{1}{\sqrt{2}} \sin\psi, \; e_3 = \cos\psi. \tag{28}$$

From Eqs (28) it is easy to see that the rotation axis is lying in the $(1\bar{1}0)$ plane, ψ being the angle between the rotation axis and the [001] direction.

Using Eqs (4), (19), (20) and (28) we have

$$W_{13}^{\alpha} = \frac{1}{\sqrt{6}} [-\sin\psi\cos\psi + (\sqrt{2} + \sin\psi\cos\psi)\cos\varphi^{\alpha} + (\sqrt{2}\cos\psi - \sin\psi)\sin\varphi^{\alpha}],$$

$$W_{23}^{\alpha} = \frac{1}{\sqrt{6}} [-\sin\psi\cos\psi - (\sqrt{2} - \sin\psi\cos\psi)\cos\varphi^{\alpha} + (\sqrt{2}\cos\psi + \sin\psi)\sin\varphi^{\alpha}],$$

$$W_{33}^{\alpha} = \frac{1}{\sqrt{3}} [\cos^2\psi + \sin^2\psi\cos\varphi^{\alpha} + \sqrt{2}\sin\psi\sin\varphi^{\alpha}]. \tag{29}$$

From Eqs (2) and (29) one has

$$\sum_{\beta} \tilde{P}_{33}^{\alpha\beta} = A \left[4\cos^2\psi + \frac{1}{3}(2 + \sin^2\psi) \sum_{\beta} \cos(\varphi^{\beta} - \varphi^{\alpha}) \right], \tag{30}$$

and, following the procedure from Sec. 3, we obtain

$$S^2 \sum_{\beta} \tilde{P}_{33}^{\alpha\beta} = 12AS^2 + U_0(\dot{\varphi}^{\alpha})^2, \tag{31}$$

where

$$U_0 = -\frac{1}{3}(2 + \sin^2\psi) AS^2a^2. \tag{32}$$

Inserting (29) in (3) one has for $S^2 \tilde{Q}^{\alpha\beta}$ the Eq. (15) with the coefficients $V_1 \ldots U_4$ from Appendix V.

The energy of the 109° Bloch walls, according to Eq. (III. 8), is thus

$$\sigma = \sigma_0 \sqrt{\frac{4}{3}(2 + \sin^2\psi)} \int_0^{2\pi} [+v_1 \sin\psi + v_2 \sin 2\psi + v_3 \sin 3\psi +$$

$$+ v_4 \sin 4\varphi + u_1 \cos\varphi + u_2 \cos 2\varphi + u_3 \cos 3\varphi + u_4 \cos 4\varphi -$$

$$- u_1 - u_2 - u_3 - u_4]^{1/2} d\varphi \tag{33}$$

where the coefficients v_i and u_i are defined by Eqs (18) with $V_1 \ldots U_4$ from Appendix V, and σ_0 is given by Eq. (27).

The integral in Eq. (33) was calculated numerically for ψ changing by 1° from 0° to 90°. The results are given by the curve σ/σ_0 in Fig. 7.

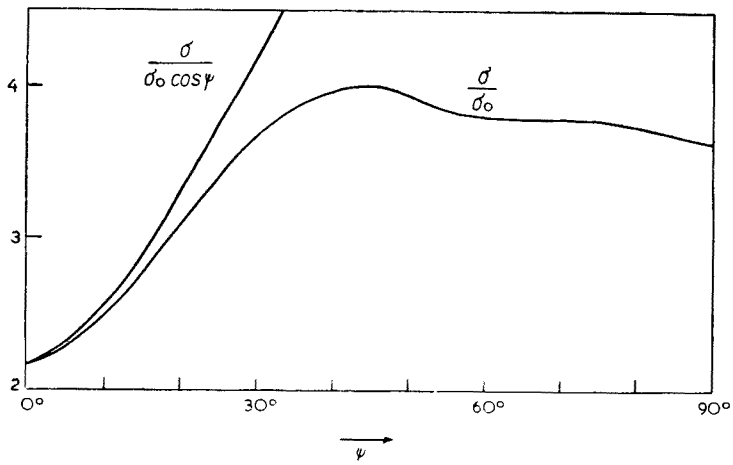

Fig. 7. Relative 109° Bloch walls energy per unit area σ/σ_0 and total Bloch walls energy $\sigma/\sigma_0 \cos\psi$ *vs* Bloch walls orientation ψ

Discussion of results

In determining the energetically most favourable Bloch walls within each class, one should minimize the total energy of the Bloch walls rather than the mere energy density σ. This problem, however, is generally insoluble, as the surface area of a Bloch wall depends in a quite complicated way on the type of the domain structure which, in turn, is determined by the shape and crystallographic orientation of the crystal. Even if neglecting surface effects (closure domains, demagnetizing field produced by free magnetic poles on the crystal surface, *etc.*) and restricting the considerations to the main domains inside the crystal, there is still the difficult problem of passing from one domain structure to another, which seldom can be achieved within the same Bloch wall class. Besides, the domain width should actually be includet (as a minimizing parameter) in the considerations, since it is the minimum energy of the entire domain structure rather than of any particular Bloch wall which is relevant to the problem of stability. Hence, considerations of the type carried through in [1], [2], [3] are necessarily of limited validity, as none of the factors mentioned above is accounted for in the calculations. None the less, we shall show that even within these limitations the results depend essentially upon whether or not the polarization is assumed to be the same for all Bloch walls.

Following [2], [3], let us consider three particular cases of minimizing the total Bloch wall energy corresponding to the three Bloch wall classes examined in the present paper. Assume the plate-like sample to be cut parallel to the (010) or (110) plane, respectively for

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the bcc or fcc lattice. Assume further a periodic domain structure whose (plate-like) domains are magnetized alternately in the directions [001], [100] for the bcc sample, and [1$\bar{1}$1], [1$\bar{1}\bar{1}$] or [1$\bar{1}$1], [$\bar{1}$11] for the fcc sample. As these directions are perpendicular to the crystal axes [010] and [110], respectively, the domains produce no magnetic poles on the upper and lower surfaces of the respective samples (poles produced on lateral surfaces are neglected, the sample being assumed to be sufficiently thin). The Bloch walls of these domain structures belong respectively to the 90°, 71° and 109° Bloch wall classes. For $\psi = 0$, the walls are perpendicular to the plane of the sample, their surface area D_0 (assumed to be the

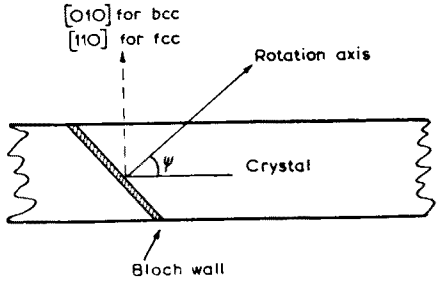

Fig. 8. Position of the Bloch wall of one of the considering classes in the plate-like crystal sample

same for all Bloch walls) being smallest. The corresponding surface area D for any ψ is thus $D = D_0/\cos\psi$ (see Fig. 8). Since in this simple model the total energy of the domain structure is simply the sum of the total energies of the Bloch walls, the problem reduces to minimizing the quantity $\sigma \cdot D$ or, equivalently, the relative energy

$$\frac{\sigma D}{\sigma_0 D_0} = \frac{\sigma}{\sigma_0 \cos\psi}, \tag{34}$$

the angle ψ being the only minimizing parameter. The curves for this expression corresponding to the three Bloch wall classes are drawn in Figs. 4, 6 and 7.

When comparing these curves with those obtained in [2], [3] for identically polarized Bloch walls, one sees that in our case all minima correspond to $\psi = 0°$. Thus, the energetically most favoured Bloch walls appear to be those which are perpendicular to the plane of the sample, *i. e.*, to the (010) and (110) planes for the bcc and fcc lattice respectively. Since $\psi = 0°$ implies $\Phi = 2\pi - \Phi = \pi$, the magnetization vectors of all the domains lie symmetrically on the rotation cone.

The difference between our results and those obtained in [2], [3] is apparently due to the fact that σ as used in [2], [3] is the energy (per cm^2) of a single Bloch wall for a rotation of the magnetization vector from $\varphi = 0$ to $\varphi = \Phi$ (or *vice versa*), and that the periodic domain structure is composed of such walls only, whereas in our case σ is the energy of all walls that may occur for φ changing from 0 to 2π. Since both approaches leads to different results ($\psi \neq 0$ and $\Phi < \pi$ was obtained in [2], [3]), it is a matter of experimental evidence in providing the justification for the applicability of either model.

Strangely enough, both approaches seem to have experimental support. In [2], 90° Bloch walls have been observed (in iron whiskers) which were not perpendicular to the (010)

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surface of the sample ($\psi = 23°$), although no similar experimental evidence is known for 71° and 109° Bloch walls in fcc crystals. On the other hand, it is a rather well established fact that, at least in bulk materials, the 90°, 71° and 109° Bloch walls are usually perpendicular to the (010) or (110) crystal surfaces (*e. g.*, [14], [15], [16]). Furthermore, there is a number of papers in which the polarization of Bloch walls in various domain structures has been examined and found to alternate from wall to wall (*e. g.*, [17], [18], [6]), which calls for the definition of σ as used in our paper. It would thus seem that our approach is applicable to the typical domain structure as usually observed in ferromagnets, in which the magnetization vector on passing through Bloch walls rotates in the same sense (screw-like) throughout the crystal, while the model studied in [2], [3] describes quite particular domain structures that may occur in specific samples and/or under specific conditions (small or thin crystals of particular shape and crystallographic orientation, local irregularities in domain structures in large crystals, *etc.*).

There appears to be an additional relative minimum for the 71° Bloch walls, for $\psi = 35°$ (see Fig. 6), which corresponds to a wall inclined at an angle 55° to the (110) crystal surface. Walls of that type have not yet been observed, probably because of their poor stability (weak minimum).

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APPENDIX I

In calculating Eq. (12) one has to evaluate the sum

$$\sum_{\beta} (e_\mu \varrho_\mu^\beta)^2 \tag{I.1}$$

where e_μ are direction cosines of the rotation axis and ϱ_μ^β denotes the μ-component of the space vector pointing from a given lattice site to its neighbour β in the bcc or fcc lattice.

As $e_\mu \varrho_\mu^\beta$ is a scalar product, the sum (I.1) should not depend on how one fixes the coordinate system. Let us fix the coordinate system as in Figs 3 and 5 for the bcc and the fcc respectively.

The sum can be written in the form

$$\sum_{\beta} (e_\mu \varrho_\mu^\beta)^2 = e_1^2 \sum_{\beta} (\varrho_1^\beta)^2 + e_2^2 \sum_{\beta} (\varrho_2^\beta)^2 + e_3^2 \sum_{\beta} (\varrho_3^\beta)^2 + \\ + 2e_1 e_3 \sum_{\beta} \varrho_1^\beta \varrho_3^\beta + 2e_1 e_2 \sum_{\beta} \varrho_1^\beta \varrho_2^\beta + 2e_2 e_3 \sum_{\beta} \varrho_2^\beta \varrho_3^\beta \tag{I.2}$$

and the sums over β can be carried out for both the bcc and fcc lattice. According to Figs. 3 and 5 we have in both cases

$$\sum_{\beta} \varrho_\mu^\beta \varrho_\nu^\beta = \delta_{\mu\nu} 2a^2 \tag{I.3}$$

where a is the lattice constant.

Since $e_\mu^2 = 1$, we obtain finally

$$\sum_{\beta} (e_\mu \varrho_\mu^\beta)^2 = 2a^2 \tag{I.4}$$

for any rotation axis.

APPENDIX II

The coefficients $V_1 \ldots U_4$ used in Sec. 3 are as follows

$$V_1 = KS^2\left(S-\frac{1}{2}\right)^2 \sin\psi\cos^2\psi\left[\frac{3}{4}-2\cos^2\psi+\frac{21}{16}\cos^4\psi\right],$$

$$V_2 = KS^2\left(S-\frac{1}{2}\right)^2 \sin\psi\cos^2\psi\left[-\frac{1}{4}+\frac{5}{4}\cos^2\psi-\frac{21}{16}\cos^4\psi\right],$$

$$V_3 = KS^2\left(S-\frac{1}{2}\right)^2 \sin\psi\cos^2\psi\left[-\frac{1}{4}+\frac{9}{16}\cos^4\psi\right],$$

$$V_4 = KS^2\left(S-\frac{1}{2}\right)^2 \sin\psi\cos^2\psi\left[\frac{1}{8}-\frac{1}{8}\cos^2\psi-\frac{3}{32}\cos^4\psi\right],$$

$$U_1 = KS^2\left(S-\frac{1}{2}\right)^2 \cos^2\psi\left[\frac{3}{4}-\frac{11}{4}\cos^2\psi+\frac{53}{16}\cos^4\psi-\frac{21}{16}\cos\psi^6\right],$$

$$U_2 = KS^2\left(S-\frac{1}{2}\right)^2 \cos^4\psi\left[\frac{1}{8}-\frac{5}{8}\cos^2\psi+\frac{21}{32}\cos^4\psi\right],$$

$$U_3 = KS^2\left(S-\frac{1}{2}\right)^2 \cos^2\psi\left[\frac{1}{4}+\frac{1}{4}\cos^2\psi-\frac{5}{16}\cos^4\psi-\frac{3}{16}\cos^6\psi\right],$$

$$U_4 = KS^2\left(S-\frac{1}{2}\right)^2\left[\frac{1}{8}-\frac{1}{4}\cos^2\psi+\frac{1}{8}\cos^6\psi+\frac{3}{128}\cos^8\psi\right].$$

APPENDIX III

For the average energy (1) we have, according to (14), (15), (24) and (31), for all Bloch wall classes considered in this paper the general form

$$h = C' + \sum_{\alpha}\{U_0(\dot{\varphi}^{\alpha})^2 - V_1\sin\varphi^{\alpha} - V_2\sin 2\varphi^{\alpha} - V_3\sin 3\varphi^{\alpha} -$$

$$-V_4\sin 4\varphi^{\alpha} - U_1\cos\varphi^{\alpha} - U_2\cos 2\varphi^{\alpha} - U_3\cos 3\varphi^{\alpha} - U_4\cos 4\varphi^{\alpha}\}, \tag{III.1}$$

the constant C' being immaterial for further considerations.

When passing to a continuous variable one has to replace the sum over α in (III.1) by an integral

$$\sum_{\alpha} \to ma^{-3} D \int_L d\xi \tag{III.2}$$

where L is the length of the crystal in the ξ direction and D the surface area (assumed to be constant) of the crystal's cross-section perpendicular to the ξ-axis (*i. e.*, to the rotation axis). The coefficient m in formula (III.2) is equal to the number of lattice atoms in the elementary cube of the crystal lattice ($m = 2$ for the bcc and $m = 4$ for the fcc lattice).

The functional which we obtain for the average energy h of the crystal has thus the form

$$h[\varphi] = C' + ma^{-3}D \int_L \{U_0\dot{\varphi}^2 - V_1 \sin\varphi - V_2 \sin 2\varphi - V_3 \sin 3\varphi - V_4 \sin 4\varphi - U_1 \cos\varphi - U_2 \cos 2\varphi - U_3 \cos 3\varphi - U_4 \cos 4\varphi\}\, d\xi. \tag{III.3}$$

The constant C' and the coefficients $U_0, V_1, \ldots U_4$ depend only on ψ (choice of rotation axis).

Following the usual variational procedure we arrive at the first order differential equation

$$\dot{\varphi}^2 = \frac{1}{U_0}\{-V_1 \sin\varphi - V_2 \sin 2\varphi - V_3 \sin 3\varphi - V_3 \sin^4\varphi - U_1 \cos\varphi - U_2 \cos 2\varphi - U_3 \cos 3\varphi - U_4 \cos 4\varphi\} + \text{const}, \tag{III.4}$$

We demand $\dot{\varphi}^2 \geqslant 0$ for all angles φ (real solutions for all φ). This is fulfilled for

$$\text{const} \geqslant \frac{1}{U_0}[U_1 + U_2 + U_3 + U_4] \tag{III.5}$$

because in our case $\varphi = 0$ corresponds always to an easy direction and, consequently, to an absolute minimum for (III.3) as well as for the right-hand side of Eq. (III.4)[2].

Choosing the equality sign in Eq. (III.5) we get the asymptotic description of Bloch walls:

$$\dot{\varphi}^2 = \frac{1}{U_0}[-V_1 \sin\varphi - V_2 \sin 2\varphi - V_3 \sin 3\varphi - V_4 \sin 4\varphi - U_1 \cos\varphi - U_2 \cos 2\varphi - U_3 \cos 3\varphi - U_4 \cos 4\varphi + U_1 + U_2 + U_3 + U_4]. \tag{III.6}$$

The surface energy density of the Bloch is usually defined as

$$\sigma = (h_\varphi - h_0)/D \tag{III.7}$$

where h_φ is the energy evaluated by inserting the solution of the variational principle into the functional (III.3), and h_0 the energy obtained by taking in the functional φ and $\dot{\varphi}$ for the easy directions.

By using Eqs (III.3), (III.6) and (III.7) we obtain

$$\sigma = 2ma^{-3}\sqrt{U_0}\int_{\varphi_1}^{\varphi_2}[-V_1 \sin\varphi - V_2 \sin 2\varphi - V_3 \sin 3\varphi - V_4 \sin 4\varphi - U_1 \cos\varphi - U_2 \cos 2\varphi - U_3 \cos 3\varphi - U_4 \cos 4\varphi + U_1 + U_2 + U_3 + U_4]^{1/2} d\varphi \tag{III.8}$$

where for a given (single) Bloch wall the integration limits should be matched in conformity with the boundary conditions for Eq. (III.4). When calculating the sum of the energy densities for all Bloch walls contained in the interval 2π, which is the case of the present paper, φ_1 can be chosen quite arbitrarily provided $\varphi_2 = \varphi_1 + 2\pi$. For simplicity we put $\varphi_1 = 0$, $\varphi_2 = 2\pi$.

[2] This can be shown without referring to any physical arguments by examining maxima and minima of the form (3).

APPENDIX IV

The coefficients $V_1, \ldots, U_4$ used in Sec. 4.1 are defined by the formulae:

$$V_1 = -\frac{1}{9} KS^2 \left(S - \frac{1}{2}\right)^2 [\sin\vartheta - 10\sin^3\vartheta + 23\sin^5\vartheta -$$

$$-14\sin^7\vartheta + \cos\vartheta - 10\cos^3\vartheta + 23\cos^5\vartheta - 14\cos^7\vartheta],$$

$$V_2 = -\frac{1}{9} KS^2 \left(S - \frac{1}{2}\right)^2 [10\sin^3\vartheta - 24\sin^5\vartheta + 14\sin^7\vartheta +$$

$$+ 10\cos^3\vartheta - 24\cos^5 + 14\cos^7\vartheta],$$

$$V_3 = -\frac{1}{9} KS^2 \left(S - \frac{1}{2}\right)^2 [\sin\vartheta - 6\sin^3\vartheta + 11\sin^5\vartheta -$$

$$-6\sin^7\vartheta + \cos\vartheta - 6\cos^3\delta\,\vartheta + 11\cos^5\vartheta - 6\cos^7\vartheta],$$

$$V_4 = -\frac{1}{9} KS^2 \left(S - \frac{1}{2}\right)^2 [-\sin\vartheta + 2\sin^3\vartheta - 2\sin^5\vartheta + \sin^7\vartheta -$$

$$-\cos\vartheta + 2\cos^3\vartheta - 2\cos^5\vartheta + \cos^7\vartheta],$$

$$U_1 = -\frac{1}{9} KS^2 \left(S - \frac{1}{2}\right)[7\sin^2\vartheta - 35\sin^4\vartheta + 56\sin^6\vartheta -$$

$$-28\sin^8\vartheta + \sin\vartheta\cos\vartheta\,(1 - 4\sin^2\vartheta + 4\sin^4\vartheta)],$$

$$U_2 = -\frac{1}{9} KS^2 \left(S - \frac{1}{2}\right)^2 [14\cos^4\vartheta - 28\cos^6\vartheta + 14\cos^8\vartheta - 4\sin^3\vartheta\cos^3\vartheta],$$

$$U_3 = -\frac{1}{9} KS^2 \left(S - \frac{1}{2}\right)^2 [\sin^2\vartheta - 5\sin^4\vartheta + 8\sin^6\vartheta -$$

$$-4\sin^8\vartheta + \sin\vartheta\cos\vartheta\,(-1 + 4\sin^2\vartheta - 4\sin^4\vartheta)],$$

$$U_4 = -\frac{1}{18} KS^2 \left(S - \frac{1}{2}\right)^2 [-2\sin^2\vartheta + 3\sin^4\vartheta - 2\sin^6\vartheta +$$

$$+\sin^8\vartheta + 1 + \sin\vartheta\cos\vartheta\,(2 - 2\sin^2\vartheta + 2\sin^4\vartheta)],$$

where $\vartheta = \psi - \pi/4$.

APPENDIX V

The coefficients $V_1, \ldots U_4$ used in Sec. 4.2 are as follows:

$$V_1 = -\frac{1}{9\sqrt{2}} KS^2 \left(S - \frac{1}{2}\right)^2 \left[2\sin\psi + 2\sin^3\psi - \frac{29}{2}\sin^5\psi + \frac{21}{2}\sin^7\psi\right],$$

$$V_2 = -\frac{1}{9\sqrt{2}} KS^2 \left(S - \frac{1}{2}\right)^2 \left[-4\sin^3\psi + 13\sin^5\psi - \frac{21}{2}\sin^7\psi\right],$$

$$V_3 = -\frac{1}{9\sqrt{2}} KS^2 \left(S-\frac{1}{2}\right)^2 \left[2\sin\psi - 2\sin^3\psi - \frac{9}{2}\sin^5\psi + \frac{9}{2}\sin^7\psi\right],$$

$$V_4 = -\frac{1}{9\sqrt{2}} KS^2 \left(S-\frac{1}{2}\right)^2 \left[-2\sin\psi + 3\sin^3\psi + \frac{1}{2}\sin^5\psi - \frac{3}{4}\sin^7\psi\right],$$

$$U_1 = -\frac{1}{9} KS^2 \left(S-\frac{1}{2}\right)^2 \left[\sin^2\psi + \sin^4\psi - \frac{29}{4}\sin^6\psi + \frac{21}{4}\sin^8\psi\right],$$

$$U_2 = -\frac{1}{9} KS^2 \left(S-\frac{1}{2}\right)^2 \left[2\sin^2\psi - \frac{15}{2}\sin^4\psi + \frac{17}{2}\sin^6\psi - \frac{21}{8}\sin^8\psi\right],$$

$$U_3 = -\frac{1}{9} KS^2 \left(S-\frac{1}{2}\right)^2 \left[3\sin^2\psi + \sin^4\psi - \frac{19}{4}\sin^6\psi + \frac{3}{4}\sin^8\psi\right],$$

$$U_4 = -\frac{1}{9} KS^2 \left(S-\frac{1}{2}\right)^2 \left[\frac{1}{2} - 2\sin^2\psi + \frac{5}{4}\sin^4\psi + \sin^6\psi - \frac{3}{32}\sin^8\psi\right].$$

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