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SURFACE MAGNETOSTRICTION WITHIN NÉEL'S MODEL

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The aim of the present paper is to determine the surface magnetostriction in the spirit of Néel's model of the surface magnetic anisotropy. Calculations have been performed for bcc and fcc ferromagnetic crystals.

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1. Introduction

Due to a great improvement of material engineering (i.e. crystal growth technique) ultrathin layers and multilayers are now available, that causes new possibilities of research, especially for investigation of surface phenomena. One of topical questions connected with surface magnetism is the understanding of surface magnetic anisotropy.

The concept of surface magnetic anisotropy was introduced by Néel [1]. Néel's theoretical study was phenomenological and similar to Van Vleck's approach to the bulk problem.

The basic assumptions of Néel's model are following:

(i) a system of localized spins is considered,

(ii) the same pseudodipolar interactions are responsible for both the magnetic anisotropy and the magnetostriction of a bulk sample,

(iii) though dipolar interactions are of the long range, only the nearest neighbours interactions are taken into account,

(iv) the difference between the environment (i.e., the positions of nearest neighbours) of the surface atom and those of the bulk is the source of surface magnetic anisotropy.

Because it is known that the magnetic anisotropy and the magnetostriction have the same origin, one can use Néel's model of magnetic surface anisotropy in order to determine surface magnetostriction. This is the aim of the present paper. Detailed understanding of mechanisms responsible for surface magnetostriction has been still lacking. Following Néel, the present approach assumes that the origin of the surface magnetostriction lies in the symmetry restrictions at the surface of the crystal.

2. Calculations

Our calculations have been performed in a way similar to that used by Bruno for hcp cobalt [2]. In this model of localized moments, the magnetocrystalline energy is assumed to be a sum of two-body terms of the following form:

$$E_{ij} = g_2(r)P_2(\cos\phi) + g_4(r)P_4(\cos\phi) + \ldots, \tag{1}$$

where r is the distance between atoms i and j, and ϕ is the polar angle between the ij direction and the common direction of the spins S_i and S_j, which are bound together by the exchange interaction, P_2 and P_4 are Legendre polynomials.

The lowest-order magnetostriction is obtained by keeping only the first order

$$g_2(r) = p + m\delta r. \tag{2}$$

Since $g_2(r)$ must decrease faster than $1/r^3$ [1] we also make the assumption that only the nearest neighbours need to be considered.

Within the above model two cases have been considered:

(i) — case A — a single crystal ferromagnet of face centred cubic structure (e.g., Ni with easy axis {111} direction), and

(ii) — case B — a single crystal ferromagnet of body centred cubic structure (e.g., Fe with easy axes along the cube edges).

In both cases samples have been cut this way that the {001} axes are perpendicular to the crystal surface plane.

The calculations starts with the magnetoelastic energy of the form [2]:

$$E_{\mathrm{ME}} = (1/2)\sum{}' \left[2p \left(\sum_{i,j,k} \alpha_i\alpha_k\beta_i\beta_j\varepsilon_{jk} - \sum_{i,j,k,l} \alpha_i\alpha_j\alpha_k\alpha_l\beta_i\beta_l\varepsilon_{jk} \right) + mr \left(\sum_{i,j,k,l} \alpha_i\alpha_j\alpha_k\alpha_l\beta_i\beta_l\varepsilon_{jk} - (1/3)\sum_{ij} \alpha_i\alpha_j\varepsilon_{ij} \right) \right], \tag{3}$$

where $\sum'$ means a sum over the nearest neighbours, ε_{ij} are the components of the strain tensor, β_i are the direction cosines of the magnetization and α_i are the direction cosines of the considered neighbour.

Introducing notation $S_{ijkl} = \sum{}'\alpha_i\alpha_j\alpha_k\alpha_l$ one obtains

$$E_{\mathrm{ME}} = p \left(\sum_{i,j,k} S_{ik}\beta_i\beta_j\varepsilon_{jk} - \sum_{i,j,k,l,} \beta_i\beta_l S_{ijkl}\varepsilon_{jk} \right) + (mr/2) \left(\sum_{i,j,k,l} \beta_i\beta_l S_{ijkl}\varepsilon_{jk} - (1/3)\sum_{i,j} \varepsilon_{ij}S_{ij} \right). \tag{4}$$

From symmetry considerations for atoms on the surface it follows that only a few S's are not equal to zero. They are following:

— case A —

$$S_{11} = S_{22} = 3, \quad S_{33} = 2, \quad S_{1111} = S_{2222} = 3/2,$$

$$S_{3333} = 1; \quad S_{1122} = 1, \quad S_{2233} = S_{1133} = 1/2; \tag{5a}$$

— case B —

$$S_{11} = S_{22} = S_{33} = 4/3, \quad S_{1111} = S_{2222} = S_{3333} = 4/9,$$

$$S_{1122} = S_{2233} = S_{1133} = 4/9. \tag{5b}$$

Thus, the magnetoelastic energy density can be written as

$$E_{\mathrm{ME}}/V = B_{ijkl}\beta_i\beta_j\varepsilon_{kl} = M_{ijkl}\beta_i\beta_j\sigma_{kl} \tag{6}$$

where V is volume and B_{ij} (or M_{ij}) (in Voigt notation) are the magnetoelastic tensor components taking for the surface layer the following form:

$$B_{11} = n_s\,[p(S_{11} - S_{1111}) + (mr/2)S_{1111} - (mr/6)S_{11}]\,,$$

$$B_{22} = n_s\,[p(S_{22} - S_{2222}) + (mr/2)S_{2222} - (mr/6)S_{22}]\,,$$

$$B_{33} = n_s\,[p(S_{33} - S_{3333}) + (mr/2)S_{3333} - (mr/6)S_{33}]\,,$$

$$B_{12} = n_s\,[(mr/2 - p)S_{1122} - (mr/6)S_{22}]\,,$$

$$B_{21} = n_s\,[(mr/2 - p)S_{1122} - (mr/6)S_{11}]\,,$$

$$B_{13} = n_s\,[(mr/2 - p)S_{1133} - (mr/6)S_{33}]\,,$$

$$B_{31} = n_s\,[(mr/2 - p)S_{1133} - (mr/6)S_{11}]\,,$$

$$B_{23} = n_s\,[(mr/2 - p)S_{2233} - (mr/6)S_{33}]\,,$$

$$B_{32} = n_s\,[(mr/2 - p)S_{2233} - (mr/6)S_{22}]\,,$$

$$B_{44} = n_s\,[(p/4)(S_{11} + S_{33}) + (mr/2 - p)S_{1133}]\,,$$

$$B_{55} = n_s\,[(p/4)(S_{22} + S_{33}) + (mr/2 - p)S_{2233}]\,,$$

$$B_{66} = n_s\,[(p/4)(S_{11} + S_{22}) + (mr/2 - p)S_{1122}]\,, \tag{7}$$

where n_s is the number of atoms per unit area.

If we assume that parameters p and mr for the surface are the same as for the bulk and that they are equal to those given by Néel [1], i.e. $p = 1.33 \times 10^{-16}$ erg and $mr = 7.64 \times 10^{-16}$ erg, we obtain the following values of components B_{ij}:

— case A —

$$B_{11} = B_{22} = n_s\,[(3/2)p + (1/4)mr] = 0.71 \text{ erg/cm}^2,$$

$$B_{33} = -2B_{13} = n_s\,[p + (1/6)mr] = 0.42 \text{ erg/cm}^2,$$

$$B_{12} = B_{21} = -n_s p = -0.21 \text{ erg/cm}^2,$$

$$B_{31} = -B_{11} - B_{12},$$

$$B_{44} = B_{55} = n_s\,[(3/4)p + (1/4)mr] = 0.47 \text{ erg/cm}^2,$$

$$B_{66} = n_s(p + mr)/2 = 0.72 \text{ erg/cm}^2; \tag{8a}$$

— case B —

$$B_{11} = B_{22} = B_{33} = (8/9)n_s p,$$

$$B_{12} = B_{21} = B_{13} = B_{31} = B_{32} = B_{23} = -(4/9)n_s p,$$

$$B_{44} = B_{55} = B_{66} = (2/9)n_s(p + mr). \tag{8b}$$

From the formulae (8a) and (8b) it results that for the case A symmetry at the surface is no longer cubic (it turns into uniaxial), while for the case B symmetry at the surface remains cubic.

The magnetostriction is obtained by minimising the magnetoelastic energy and elastic energy with respect to ε_{ij}. One obtains, for the direction (γ_i) [2]:

$$\lambda = \lambda_A \left[(\beta_1\gamma_1 + \beta_2\gamma_2)^2 - (\beta_1\gamma_1 + \beta_2\gamma_2)\beta_3\gamma_3\right] + \lambda_B \left[(1-\beta_3^2)(1-\gamma_3^2)\right.$$
$$\left.-(\beta_1\gamma_1 + \beta_2\gamma_2)^2\right] + \lambda_C[(1-\beta_3^2)\gamma_3^2 - (\beta_1\gamma_1 + \beta_2\gamma_2)\beta_3\gamma_3]$$
$$+\lambda_D(\beta_1\gamma_1 + \beta_2\gamma_2)\beta_3\gamma_3, \tag{9}$$

with λ_A, λ_B, λ_C and λ_D, the surface magnetostriction constants, given by

$$\lambda_A = Z^{-1}\left[(c_{11}+c_{12})(2B_{11}+B_{12}) - c_{12}(B_{11}+2B_{12}+3B_{13})\right],$$

$$\lambda_B = Z^{-1}\left[(c_{11}+c_{12})(B_{11}+2B_{12}) - c_{12}(2B_{11}+B_{12}+3B_{13})\right],$$

$$\lambda_C = 3Z^{-1}\left[(c_{11}+c_{12})B_{13} - c_{12}(B_{11}+B_{12})\right],$$

$$\lambda_D = (1/4)(\lambda_A + \lambda_C) + (1/2)(B_{44}/c_{44}),$$

$$Z = (c_{11}-c_{12})(c_{11}+2c_{12}), \tag{10}$$

where c_{ik} are the elastic constants and B_{ik} are the magnetoelastic tensor components (in Voigt notation). Values of the magnetoelastic tensor component

$$M_{11} = [(c_{11}-c_{12})(c_{11}+2c_{12})]^{-1}\left[(c_{11}+c_{12})B_{11} - c_{12}(B_{12}+B_{13})\right] \tag{11}$$

for polycrystalline nickel measured experimentally [3] are equal to $(10\text{–}90)\times10^{-6}$ nm, whereas M_{11} calculated within our model is equal to 6.7×10^{-6} nm.

3. Conclusion

The model of the magnetostriction based on Néel's assumption for surface magnetic anisotropy indicates that values of the magnetoelastic tensor components are different at the surface and inside the crystal. Mere existence of the surface, i.e. lack of several nearest neighbours for the surface layer atoms, suffices for changes in values of the magnetoelastic tensor components. In our opinion mere existence of the surface is an origin in part of the surface magnetostriction.

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