Materials Science-Poland, Vol. 26, No. 4, 2008

Pseudodipolar model of surface magnetostriction for thin layers with roughness

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An effective magnetostriction model for monocrystalline thin films of cubic structure has been presented. The film roughness was simulated by cubicoidal steps on surface repeated in the plane with a constant period. In order to describe a magnetoelastic energy, a pseudodipolar spin–spin interaction was considered. Lattice summations of strain dependent energy contribution were performed symbolically. A significant difference of magnetoelastic energy compared with the film interior was observed only in the first atomic layer at the surface. An effective pseudodipolar magnetostriction constant λ^{eff} for rough film was determined by estimating the volume of surface region and considering the magnetostriction data for bulk material. Thickness dependence of λ^{eff} for bcc Fe film has been presented and compared with magnetic dipolar contribution.

Key words: *magnetic thin layer; surface magnetostriction; surface roughness; pseudodipolar interactions*

1. Introduction

A concept of surface magnetostriction is a natural consequence of Neel's idea of surface magnetic anisotropy [1] evidenced experimentally by means of ferromagnetic resonance (FMR) [2]. The surface magnetostriction was observed for the first time in multilayers with strain modulated ferromagnetic resonance technique (SMFMR) [3]. Changes of the effective magnetostriction constants with film thickness were attributed to varying ratio of the number of surface atoms to the total population of atoms in the material. Theoretical predictions of dipolar and electronic contributions to the surface magnetostriction (within Draaisma–de Jonge [4] and Bruno models [5], respectively) have been reported in papers [6, 7]. Non-epitaxial growth of metallic films creates surface roughness which should be taken into account while considering experimental magnetostriction data [8, 9]. We propose a simple theoretical model predicting the effective magnetostriction constant values of rough films based on the values for the bulk material.

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2. Pseudodipolar interactions

We consider fully localized spins coupled via effective interaction represented by pseudodipolar term, which describes both anisotropic exchange energy and single-ion anisotropy one. [10]. Pseudodipolar Hamiltonian takes the form similar to that for magnetic dipolar interactions:

$$H_{\mathrm{A}}^{(i,j)} = J_{\mathrm{A}}\left(|\,\mathbf{r}^{(i,j)}\,|\right)\cdot\left(S_z^{(i)}S_z^{(j)} - \frac{1}{3}\mathbf{S}^{(i)}\cdot\mathbf{S}^{(j)}\right) \tag{1}$$

$S_z^{(i)}$ and $S_z^{(j)}$ are the components of spins i and j parallel to the line connecting these two spins; $\mathbf{r}^{(i,j)}$ is the vector describing a relative position of spins, $J_{\mathrm{A}}(|\mathbf{r}^{(i,j)}|)$ is an exchange integral value at a distance $|\mathbf{r}^{(i,j)}| \equiv r^{(i,j)}$. In the case of single-ion magnetocrystalline anisotropy $S^{(i)} \equiv S^{(j)}$ and $J_{\mathrm{A}}(|\mathbf{r}^{(i,j)}|)$ has a meaning of a radial function which describes the strength of magnetocrystalline anisotropy for a given interatomic distance. Hamiltonian (1) can be written in a tensor-like form:

$$H_{\mathrm{A}}^{(i,j)} = J_{\mathrm{A}}(r^{(i,j)})G_{kl}^{(i,j)}S_k^{(i)}S_l^{(j)}; \qquad G_{kl}^{(i,j)} = \frac{x_k^{(i,j)}x_l^{(i,j)}}{(r^{(i,j)})^2} - \frac{1}{3}\delta_{kl} \tag{2}$$

and then can be transformed into a semi-classical notation:

$$H_{\mathrm{A}}^{(i,j)} = J_{\mathrm{A}}(r^{(i,j)})\,|\,S\,|^2\;G_{kl}^{(i,j)}\frac{S_k^{(i)}}{|\,S\,|}\frac{S_l^{(j)}}{|\,S\,|} = J_A(r^{(i,j)})\,|\,S\,|^2\;G_{kl}^{(i,j)}\alpha_k^{(i)}\alpha_l^{(j)} \tag{3}$$

where $\alpha_k^{(i)}$, $\alpha_l^{(j)}$ are the direction cosines of spins (i) and (j) and $|S|$ is an effective value of the spin. Thus, a contribution to the density of the second-order anisotropy energy could be expressed as

$$u_{\mathrm{A}}^{(i,j)} = A_{kl}^{(i,j)}\alpha_k^{(i)}\alpha_l^{(j)}; \qquad A_{kl}^{(i,j)} = \frac{1}{2}\frac{J_{\mathrm{A}}(r^{(i,j)})\,|\,\mathrm{S}\,|^2}{V_{\mathrm{spin}}}G_{kl}^{(i,j)} \tag{4}$$

where V_{spin} is a volume per one spin. The factor 1/2 has been applied in Eq. (4) to avoid double summation in further calculations of the total energy of the system. Since magnetoelastic energy results from a strain (ε_{mn}) dependence of anisotropy energy, its density may be described by means of the fourth-rank tensor $B_{klmn}^{(i,j)}$:

$$u_{\mathrm{ME}}^{(i,j)} = B_{klmn}^{(i,j)}\alpha_k^{(i)}\alpha_l^{(j)}\varepsilon_{mn}; \qquad B_{klmn}^{(i,j)} = \frac{\partial A_{kl}^{(i,j)}}{\partial\varepsilon_{mn}} = \frac{1}{2}\frac{|\,S\,|^2}{V_{\mathrm{spin}}}\frac{\partial}{\partial\varepsilon_{mn}}\left[J_{\mathrm{A}}r^{(i,j)}G_{kl}^{(i,j)}\right] \tag{5}$$

Further recalculations allow one to express the tensor $B_{klmn}^{(i,j)}$ by two dimensionless tensors $b_{klmn}^{\mathrm{J}\,(i,j)}$ and $b_{klmn}^{\mathrm{P}\,(i,j)}$:

$$B_{klmn}^{(i,j)} = \frac{1}{2}\frac{|\mathrm{S}|^2}{V_{\mathrm{spin}}}\left[J_{\mathrm{A}} b_{klmn}^{\mathrm{J}(i,j)} + P_{\mathrm{A}} a_0 b_{klmn}^{\mathrm{P}(i,j)}\right];$$
$$b_{klmn}^{\mathrm{J}(i,j)} = \frac{\partial G_{kl}^{(i,j)}}{\partial \varepsilon_{mn}} \quad \text{and} \quad b_{klmn}^{\mathrm{P}(i,j)} = \frac{x_m^{(i,j)} x_n^{(i,j)}}{r^{\mathrm{NN}} a_0} \cdot G_{kl}^{(i,j)} \tag{6}$$

The parameters J^A and J^P stand for the value and the spatial derivative of the radial function $J_{\mathrm{A}}(r^{(i,j)})$ in the distance of nearest neighbours r^{NN}, respectively, when pseudodipolar interactions are limited to the first coordination zone (a_0 is the lattice constant of cubic crystalline structure).

In order to obtain the total value of local density of magnetoelastic energy for *i*th spin site, lattice summations over index *j* have been performed analytically within the first coordination zone. Calculations have been made for the case of saturation ($\alpha_k^{(i)} \equiv \alpha_k^{(j)}$). The results show that only in the first atomic layer at the surface the magnetoelastic energy differs from that in the film interior. Regarding bcc films, the values of all components of dimensionless tensors $b_{klmn}^{\mathrm{J}(i,j)}$ and $b_{klmn}^{\mathrm{P}(i,j)}$ in the surface layer are twice smaller than those in the bulk region (whereas in the case of fcc structure such relations are more complex). This means that magnetostriction of bcc films is characterized by a magnetoelastic tensor of the cubic symmetry both in the interior and at the surface.

3. Effective magnetostriction

Minimization of magnetoelastic and elastic energies, described by means of magnetoelastic tensor and elastic constants, respectively, leads to the calculation of magnetostriction constant λ (for a given direction). This dimensionless quantity is a simple measure of relative strain induced by applying a saturation magnetic field. The results of calculations of the B_{klmn} tensor (presented in the previous section) give a very simple relation between magnetostriction constants obtained for bulk material (λ^{v}) and flat surface region (λ^{s}) in the case of the bcc structure: $\lambda^{\mathrm{s}} = \lambda^{\mathrm{v}}/2$, both for [100] and [001] directions, i.e. in-plane and perpendicular to the plane, respectively.

In order to calculate the effective magnetostriction constant for a rough thin layer, it is necessary to estimate the fraction of atoms situated on the surface. The object of our investigations was a single magnetic film of a thickness *t* with surfaces in the form of cubicoidal steps of the depth σ and size ξ, repeated in the plane with the space period *q* (Fig. 1). Considering the volume of surface region (of the thickness *h* equal to a half of the lattice constant a_0) an effective magnetostriction constant λ^{eff} of rough film could be expressed as follows:

$$\lambda^{\mathrm{eff}} = \lambda^{\mathrm{v}} + \lambda^{\mathrm{surf}}\frac{2}{t}; \qquad \lambda^{\mathrm{surf}} = \left(\lambda^{\mathrm{s}} - \lambda^{\mathrm{v}}\right) h\left(1 + \frac{4\sigma\xi}{q^2}\right) \tag{7}$$

under the assumption: $\sigma << t$; λ^{surf} is the surface magnetostriction constant (in [ppm·nm]) for a rough surface.

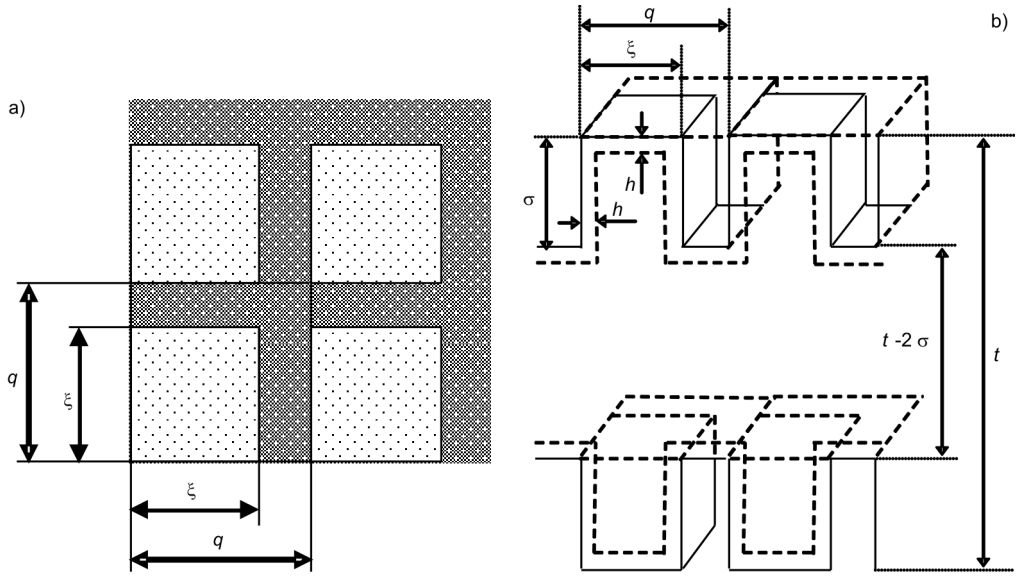

Fig. 1. Scheme of the film roughness model:
a) projection from the top, b) a perspective view of the surface

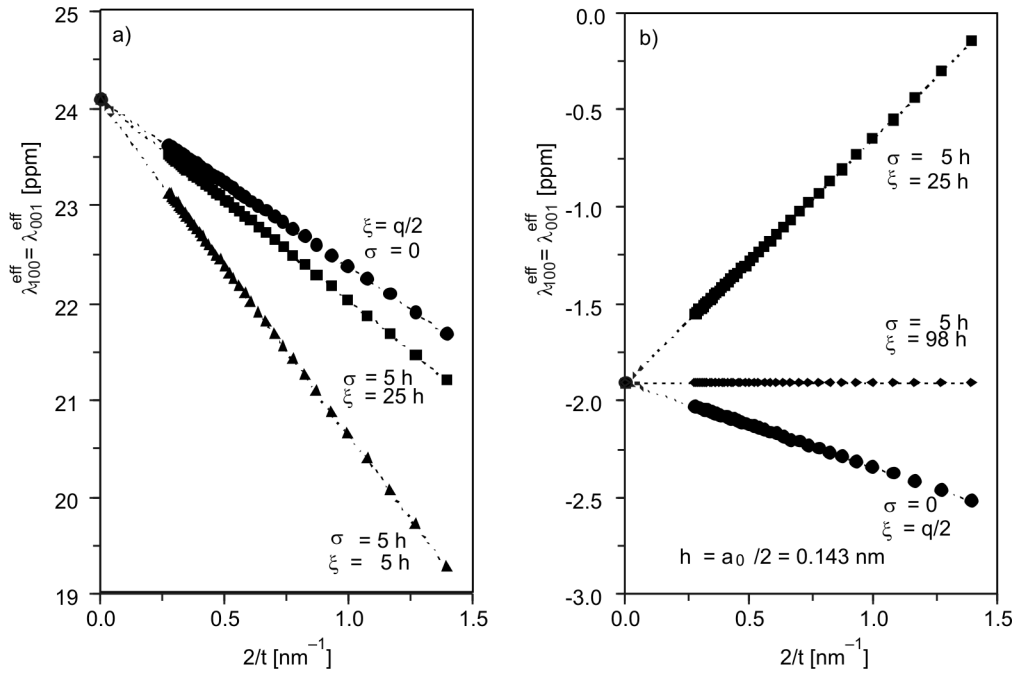

Fig. 2. Dependence of the effective magnetostriction constant for ideal and rough films on the reciprocal film thickness: a) pseudodipolar model, b) magnetic dipolar contribution

In Figure 2a, a linear dependence of the effective magnetostriction constant (Eq. (7a)) on the reciprocal film thickness is shown for the case of the bcc Fe structure ($\lambda^{v} = 24.1$ ppm, $h = a_0/2 = 0.143$ nm). We point to a significant reduction of magnetostriction for a small ξ size of steps (huge roughness area; negative value of the surface magnetostriction constant) in comparison to the case of flat surface ($\sigma = 0$).

The magnetic dipolar contribution to the in-plane magnetostriction constant of the bcc Fe film is shown in Fig. 2b. Appropriate calculations were based on models described in [6, 11, 12]. The surface roughness was represented by oblate ellipsoids (of semiaxes $\xi = q/2 >> \sigma/2$) in order to simplify the estimation of demagnetization energy. In this case, the effective dipolar magnetostriction constant is given by:

$$\lambda_{\mathrm{dip}}^{\mathrm{eff}} = \lambda_{\mathrm{dip}}^{\mathrm{v}} + \lambda_{\mathrm{dip}}^{\mathrm{surf}} \frac{2}{t}; \qquad \lambda_{\mathrm{dip}}^{\mathrm{surf}} = \left(\lambda_{\mathrm{dip}}^{\mathrm{s}} - \lambda_{\mathrm{dip}}^{\mathrm{v}}\right) h + \lambda_{\mathrm{dip}}^{0\mathrm{r}} \frac{\pi}{4} \frac{\sigma^2}{\xi} \tag{8}$$

where $\lambda_{\mathrm{dip}}^{\mathrm{v}} = -1.91$ ppm and $\lambda_{\mathrm{dip}}^{\mathrm{s}} = -4.93$ ppm denote dipolar magnetostriction constants for internal and flat surface regions, respectively [12]. The magnetostriction constant $\lambda_{\mathrm{dip}}^{0\mathrm{r}} = 15.1$ ppm describes the influence of the magnitude of the roughness being defined as:

$$\lambda_{\mathrm{dip}}^{0\mathrm{r}} = \frac{\pi \mu_0 M_{\mathrm{s}}^2}{8\left(\mathrm{c}_{11} - c_{12}\right)} \tag{9}$$

following the model developed in [11]. M_{s} is the saturation magnetization, μ_0 – magnetic permeability of the vacuum and c_{11}, c_{12} – elastic constants. The dipolar contribution to the magnetostriction of the Fe film interior is about 8% with respect to electronic (pseudodipolar) one, whereas surface dipolar contribution is more significant – ca. 25%. Results presented in Fig. 2b show that roughness tends to compensate the dipolar surface magnetostriction.

4. Conclusions

Our model, based on pseudodipolar interactions of localized spins, relates the surface magnetostriction parameters of thin films to the magnetostriction constants of bulk material. We have shown that electronic contribution to the surface magnetostriction of bcc Fe monocrystalline films increases with increasing surface roughness (fine steps of high surface density). It results in significant reduction of the effective magnetostriction in the case of very thin layers. We also have proven that magnetic dipolar contribution to the surface magnetostriction is not negligible. However, the surface roughness could partially compensate this contribution due to the opposite sign of surface magnetostriction constant for flat and rough parts of the surface, respectively. The energy of long range magnetic dipolar interactions depends both on

the volume of roughness region and the roughness shape. In a more advanced approach, a continuous magnetized medium should be replaced by a discrete system of magnetic moments of atoms forming given structure. A summation of the energy of long range dipolar interactions should be performed over the whole structure what makes such procedure extremely time-consuming. Various directions of epitaxial growth of real films and their possible polycrystallinity as well as the influence of a kind of substrate seem to be essential questions in further development of our magnetostriction model what will enable a reliable comparison with experimental data.

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Received 7 May 2007
Revised 6 October 2007