

Theory of roughness-induced anisotropy in ferromagnetic films: The dipolar mechanism

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(Received 7 January 1999)

When ferromagnetic films are grown on stepped surfaces, or rough surfaces upon which there is a preferred direction, additional magnetic anisotropy associated with the presence of the roughness is found in experiments. This paper presents the theory of the contribution of one mechanism to this anisotropy, that is associated with the roughness-induced increase in magnetic dipolar energy. When the film surface profiles are modulated, the magnetization of the film fluctuates in direction, thus generating stray dipolar fields. The energy stored in such fields depends on the angle between the mean magnetization, and the preferred axis of the modulated surface profile. We present explicit calculations for various models of films on stepped surfaces.

[S0163-1829(99)00218-0]

I. INTRODUCTION

There is currently great interest in the properties of very thin ferromagnetic films, possibly incorporated into magnetic multilayers or superlattice structures. Applications of such materials to magnetic recording have been realized recently, and such structures may possibly lead to a generation of magnetic memories. More generally, we have here a fascinating class of magnetic materials, with unique properties which range from the well-known giant magnetoresistance, to magnetic phase diagrams that are rich and subject to control through variations in the microstructure of the multilayers.

Most theoretical studies explore the properties of idealized films, whose surfaces are perfectly smooth and flat. In fact, the ultrathin films of current interest are grown on substrates which themselves are not smooth. Even the highest quality substrate has steps, for example. One thus must inquire about the influence of steps, or more generally, of surface roughness, on the magnetic properties of such films. We note that Slonczewski¹ has argued that the presence of steps plays a critical role in the biquadratic coupling found in Fe/Cr multilayers. It appears to be the case that this mechanism indeed dominates, for some samples.²

In the recent literature, attention has been directed toward experimental studies of roughness-induced anisotropy, for ultrathin films grown on surfaces whose profile has been modulated in a unidirectional manner; a stepped substrate provides an example of such a surface.³⁻⁸ Several mechanisms have been invoked to explain such data. For example, magnetic ions which reside very close to a step reside in sites of low symmetry, and thus experience anisotropy whose character and strength differs from ions which sit on a flat region. Such ions transmit information about the anisotropy they experience by virtue of their exchange coupling to the magnetic species elsewhere in the film. Also, the presence of steps will lead to strain within the magnetic film, and through magnetoelastic coupling this can generate magnetic anisotropies in the film.

In this paper we present the theory of a third contribution to the anisotropy, and evaluate its magnitude for several models of thin films with modulated surface profiles. In a

thin film with perfectly flat surfaces, in the absence of perpendicular anisotropy, the magnetization will be constant in magnitude and direction, and parallel to the film surfaces. If the surface profiles are modulated, the direction of the magnetization within the film will wander. A consequence is that fields of dipolar character are generated both by the effective volume magnetic charge density $-\nabla \cdot \vec{M}$, and also surface charges. There is an energy density associated with these fields that is a function of the angle between the average magnetization, and the preferred direction associated with the modulated surface profile. Thus, we have a contribution to the anisotropy energy from this dipolar mechanism. To initiate such studies, we consider the simplest physical picture. We have a ferromagnetic film placed in an external dc magnetic field \vec{H}_0 parallel to its nominal surface. We consider the Zeeman, dipolar, and exchange energies in our analysis.

In Sec. II, we derive the roughness-induced anisotropy energy, for the case where the amplitude of the roughness may be assumed to be small. In Sec. III we consider a simple example: a semi infinite medium with a surface roughness corresponding to a single Fourier component. Section IV presents a sequence of numerical studies, and Sec. V concluding remarks.

II. THEORETICAL DISCUSSION

The geometry we consider is illustrated in Fig. 1. We have a ferromagnetic film, of nominal thickness D . By this we mean we have an upper surface given by $y = D/2 + \xi^>(x, z)$ where the average of $\xi^>(x, z)$ over the entire surface is zero, i.e., $\langle \xi^> \rangle = 0$. Similarly, the lowest surface is $y = -D/2 + \xi^<(x, z)$, where $\langle \xi^< \rangle = 0$. Thus, $y = D/2$ is the nominal upper surface, $y = -D/2$ the nominal lower surface, and D is the average thickness of the film.

An external dc magnetic field \vec{H}_0 is applied parallel to the z axis, located in the plane $y = 0$, parallel to the two nominal surfaces. If $\xi^>(x, z) = \xi^<(x, z) = 0$ everywhere, then the magnetization \vec{M}_0 will lie in plane, uniform in magnitude and direction, and also parallel to \vec{H}_0 . (We neglect anisotropy perpendicular to the $x-z$ plane, save for the dipolar

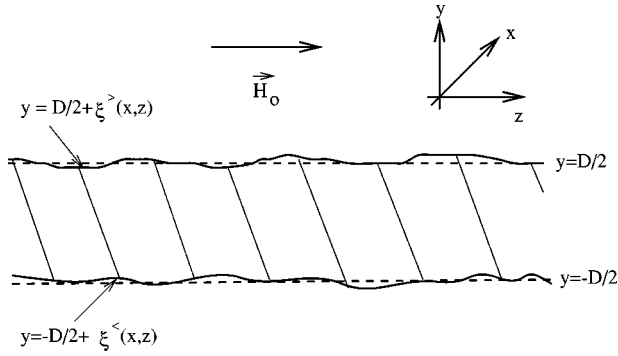


FIG. 1. Schematics of a rough film, with the applied field $\vec{H}_0 = H_0 \hat{z}$ in the plane of the nominal film of thickness D . The amplitudes $\xi^{>,<}(x, z)$ describe the upper and lower surfaces roughness.

anisotropy built into our analysis.) If either $\xi^{>}(x, z)$ or $\xi^{<}(x, z)$ are nonzero, or both are nonzero, there will be spatial variations of the magnetization direction in the film, thus \vec{M}_0 becomes a function of position, $\vec{M}_0(\vec{x})$. These spatial variations will clearly increase the Zeeman and exchange energies. In addition, there will be dipolar fields generated by the effective magnetic charge density $\rho_M(\vec{x}) = -\nabla \cdot \vec{M}_0(\vec{x})$ within the film, and also by magnetic surface charges with origin in those areas of the surface where $\vec{M}_0(\vec{x})$ has a non-zero perpendicular component. These dipolar fields increase the energy of the system as well. If the surface roughness has a directional character, say the film is grown on a stepped surface, then this energy will clearly depend on the angle θ between the preferred direction, and that of the applied magnetic field \vec{H}_0 .

In this section, we obtain expressions for these roughness-induced energy changes, within the framework of a perturbation theoretic scheme. We assume the deviation in the magnetization $\vec{M}_0(\vec{r})$ from the nominal value $\vec{M}_0 = M_0 \hat{z}$ is small, and may be calculated to first order in $\xi^{>}$ and $\xi^{<}$. With this information in hand, we may calculate the energy change of the system to second order in these quantities. This section is devoted to the basic formulation of the theory, and subsequent sections to applications.

In the presence of roughness, we write the magnetization in the form

$$\vec{M}(\vec{x}) = \left(M_0 - \frac{1}{2M_0} [m_x^2(\vec{x}) + m_y^2(\vec{x})] \right) \hat{z} + m_x(\vec{x}) \hat{x} + m_y(\vec{x}) \hat{y}, \quad (1)$$

where the quantities $m_x(\vec{x})$ and $m_y(\vec{x})$ are of first order in the amplitudes of the roughness. The energy of the system is then

$$E = -H_0 \int d^3x M_z(\vec{x}) - \frac{1}{2} \int d^3x \vec{H}_d(\vec{x}) \cdot \vec{M}(\vec{x}) + \frac{A}{M_0^2} \int d^3x \sum_{\alpha} |\vec{\nabla} M_{\alpha}|^2. \quad (2)$$

In these expressions, $\vec{H}_d(\vec{x})$ is the dipolar field generated by nonuniformities in the magnetization, produced by the roughness. The first term in Eq. (2) is the Zeeman energy,

the second is the dipolar energy, and the third is the exchange energy. The integrals are over the actual volume of the rough film. We ignore surface anisotropy, so when we generate expressions for $m_x(\vec{x})$ and $m_y(\vec{x})$, we use the boundary conditions $\hat{n} \cdot \nabla m_x = 0$, and $\hat{n} \cdot \nabla m_y = 0$ on each surface, where \hat{n} is a normal to the surface. Since, in fact, m_x and m_y are first order in the roughness amplitude, so long as we require these quantities only to lowest order, we may replace the exact boundary conditions by the four statements

$$\left. \frac{\partial m_{x,y}}{\partial y} \right|_{y=\pm D/2} = 0. \quad (3)$$

We write the total energy of the system as

$$E = -H_0 M_0 V + \Delta E, \quad (4)$$

where $-H_0 M_0 V$ is the Zeeman energy of the uniformly magnetized film, and ΔE is the change induced by the presence of the roughness. For the Zeeman term,

$$\Delta E_Z = \frac{H_0}{2M_0} \int_{\bar{V}} d^3x (m_x^2 + m_y^2), \quad (5)$$

where, since m_x and m_y are first order in the roughness, the integral is confined to the volume \bar{V} between the nominal surfaces at $\pm D/2$. We write for the change in dipolar energy, with $\vec{H}_d(\vec{x}) = h_x(\vec{x}) \hat{x} + h_y(\vec{x}) \hat{y} + h_z(\vec{x}) \hat{z}$,

$$\Delta E_D = -\frac{M_0}{2} \int_V d^3x h_z(\vec{x}) - \frac{1}{2} \int_{\bar{V}} d^3x [m_x h_x + m_y h_y]. \quad (6)$$

In the second term in this expression, both m_x and h_x are first order in the roughness amplitude, so we may integrate only over the ‘‘nominal film’’ volume \bar{V} . In the first term, since h_z is first order, we must take due account of the actual roughened surfaces, as we shall see shortly.

In regard to the exchange energy, note that

$$\begin{aligned} \int_V d^3x |\vec{\nabla} M_{\alpha}(\vec{x})|^2 &= \int_V d^3x \{ \vec{\nabla} \cdot (M_{\alpha} \vec{\nabla} M_{\alpha}) - M_{\alpha} \nabla^2 M_{\alpha} \} \\ &= - \int_V d^3x M_{\alpha} \nabla^2 M_{\alpha} + \int_S dS M_{\alpha} \hat{n} \cdot \nabla M_{\alpha} \\ &= - \int_V d^3x M_{\alpha} \nabla^2 M_{\alpha}. \end{aligned} \quad (7)$$

The integral over the film surfaces vanishes to all orders in the roughness, by virtue of our boundary condition $\hat{n} \cdot \vec{\nabla} M_{\alpha} = 0$ on the surface. We then have, with

$$h_{x,y}^{(ex)} = \frac{2A}{M_0^2} \nabla^2 m_{x,y}, \quad (8)$$

$$\Delta E_{ex} = -\frac{1}{2} \int_{\bar{V}} d^3x \left[m_x h_x^{(ex)} + m_y h_y^{(ex)} - \frac{A}{M_0^2} \nabla^2 (m_x^2 + m_y^2) \right], \quad (9)$$

where the last term has its origin in $M_z \nabla^2 M_z$. We have

$$\int_{\bar{V}} d^3x \nabla^2(m_{x,y}^2) = \int_{\bar{S}} dS \hat{n} \cdot \vec{\nabla} m_{x,y}^2 = 2 \int_{\bar{S}} dS m_{x,y} \hat{n} \cdot \vec{\nabla} m_{x,y} = 0 \quad (10)$$

by virtue of the boundary condition. Hence, the last term vanishes. Thus,

$$\Delta E_{\text{ex}} = -\frac{1}{2} \int_{\bar{V}} d^3x [m_x h_x^{(\text{ex})} + m_y h_y^{(\text{ex})}]. \quad (11)$$

Relations between various contributions noted above follow when one realizes that for the system to be in equilibrium, we must have the zero torque condition

$$\vec{M}(\vec{x}) \times \vec{H}_{\text{eff}} = 0, \quad (12)$$

where $\vec{M}(\vec{x})$ is given in Eq. (1), and the effective field sensed by the magnetization is the sum of the Zeeman field, the dipole field, and the exchange field. The contributions to the local torque to first order in the roughness amplitude read

$$\begin{aligned} \vec{M}(\vec{x}) \times \vec{H}_{\text{eff}} = & \hat{x} [H_0 m_y - M_0 (h_y + h_y^{(\text{ex})})] \\ & + \hat{y} [M_0 (h_x + h_x^{(\text{ex})}) - H_0 m_x]. \end{aligned} \quad (13)$$

We then require the relation

$$m_{x,y} = \frac{M_0}{H_0} (h_{x,y} + h_{x,y}^{(\text{ex})}). \quad (14)$$

Then notice

$$\begin{aligned} \Delta E_D + \Delta E_{\text{ex}} = & -\frac{M_0}{2} \int_{\bar{V}} d^3x h_z(\vec{x}) \\ & -\frac{1}{2} \int_{\bar{V}} [m_x (h_x + h_x^{(\text{ex})}) + m_y (h_y + h_y^{(\text{ex})})] \\ = & -\frac{M_0}{2} \int_{\bar{V}} d^3x h_z(\vec{x}) - \frac{H_0}{2M_0} \int_{\bar{V}} d^3x [m_x^2 + m_y^2]. \end{aligned} \quad (15)$$

Notice that the second term precisely cancels the Zeeman energy, so that we have quite simply

$$\Delta E = -\frac{M_0}{2} \int_{\bar{V}} d^3x h_z(\vec{x}), \quad (16)$$

where as we have emphasized earlier, the integration on the right-hand side of Eq. (16) is over the volume of the real film, with its rough surfaces.

Now in the magnetostatic approximation,

$$h_z(\vec{x}) = -\frac{\partial \Phi}{\partial z} \quad (17)$$

with Φ the magnetic potential, a quantity first order in the roughness amplitude, to leading order. Thus,

$$\Delta E = \frac{M_0}{2} \int_{\bar{V}} \frac{\partial \Phi}{\partial z} dz dy dx. \quad (18)$$

To evaluate the integration in Eq. (18), we must consider various regions. Suppose first that the roughness is confined

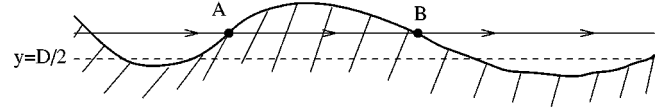
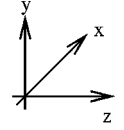


FIG. 2. A path of integration in the rough surface region.

to a finite domain of the variable z , from $-L/2$ to $L/2$. In the end we let $L \rightarrow \infty$. But for finite L , $\Phi \rightarrow 0$ as $z \rightarrow +\infty$, and $z \rightarrow -\infty$. Now suppose $\xi^>$ has the maximum (positive) value $\xi_M^>$, and a maximum negative value $-\xi_M^<$. Similarly, $\xi^<$ varies from $+\xi_M^<$ to $-\xi_M^>$. Then in the region $(D/2) - \xi_M^> > y > -(D/2) + \xi_M^<$. There is zero contribution to the integral, since we integrate continuously from $-\infty$ to $+\infty$, and Φ vanishes at the two limits for finite L .

We then concentrate on the regime where y lies between $(D/2) + \xi_M^>$, and $(D/2) - \xi_M^<$, and similarly for the lower surface. We examine this contribution with the aid of Fig. 2. For fixed x and y , we imagine the contribution by integrating in z along the solid line in the figure. We have contributions from only those positions of the solid line which lie within the film. We focus attention on the contribution from the particular line segment AB. The contribution to the integral in Eq. (18) from this segment is $[\Phi(x, y, z_B) - \Phi(x, y, z_A)] dx dy$. Now let $d\vec{S}$ be an element of (vector) surface area on the real film, using the usual convention that $d\vec{S}$ points outward from the volume bounded. Then at point B, $dS_z^{(B)} = dx dy$, while at point A, $dS_z^{(A)} = -dx dy$. Hence the contribution to the integral from this line segment is $\Phi(x, y, z_B) dS_z^{(B)} + \Phi(x, y, z_A) dS_z^{(A)}$. From this argument, one concludes that Eq. (18) may be written as

$$\Delta E = \frac{M_0}{2} \int_{\bar{S}} dS_z \Phi, \quad (19)$$

where the integral is over both surfaces of the film, upper and lower. Indeed the result of Eq. (19) follows directly from Eq. (18) by use of a general version of the divergence theorem: $\int dV \partial \Phi / \partial x_i = \int dS_i \Phi$.

If the surfaces of the film are perfectly flat, $dS_z \equiv 0$, and $\Delta E = 0$. The quantity dS_z is thus nonzero only when $\xi^>(x, z)$ and/or $\xi^<(x, z)$ are nonzero. To lowest order in the roughness, it is an elementary exercise to show that on the upper or lower surface

$$dS_z^{>,<} = \mp dx dz \frac{\partial \xi^{>,<}}{\partial z}. \quad (20)$$

When this is inserted into Eq. (19), we may simply calculate the magnetic potential Φ to first order in the roughness amplitude, evaluate it on the nominal surfaces $y = \pm D/2$, and integrate over x and z .

We thus arrive at a remarkably simple expression for the total change in energy of the system, to second order in the roughness amplitude:

$$\Delta E = -\frac{M_0}{2} \int dx dz \left[\Phi(x, D/2, z) \frac{\partial \xi^>}{\partial z}(x, z) - \Phi(x, -D/2, z) \frac{\partial \xi^<}{\partial z}(x, z) \right]. \quad (21)$$

We shall Fourier transform the various quantities which enter the above expression. For example, if $\vec{\rho}$ lies in the xz plane, and $\vec{Q} = Q_x \hat{x} + Q_z \hat{z}$, we write

$$\Phi(x, y, z) = \sum_{Q_x, Q_z} \Phi(\vec{Q}; y) e^{i\vec{Q} \cdot \vec{\rho}}, \quad (22)$$

and similarly for $\xi^{>, <}(x, z)$. Then the change in energy per surface area is

$$\frac{\Delta E}{\mathcal{A}} = \frac{iM_0}{2} \sum_{Q_x, Q_z} Q_z [\xi^>(\vec{Q}) * \Phi(\vec{Q}; D/2) - \xi^<(\vec{Q}) * \Phi(\vec{Q}; -D/2)], \quad (23)$$

where \mathcal{A} is the quantization area [$\xi^{>, <}(-\vec{Q}) = \xi^{>, <}(\vec{Q})^*$]. Our task is now to find the magnetic potential $\Phi(\vec{x})$, for the film with rough surfaces. For this purpose, we consider sinusoidally modulated surfaces for which

$$\xi^{>, <}(x, z) = \xi^{>, <}(\vec{Q}) e^{i\vec{Q} \cdot \vec{\rho}} + \text{c.c.} \quad (24)$$

(c.c. represents complex conjugate). If $\vec{b}(\vec{x}) = \vec{h}(\vec{x}) + 4\pi\vec{m}(\vec{x}) = -\nabla\Phi(\vec{x}) + 4\pi\vec{m}(\vec{x})$, we require $\nabla \cdot \vec{b}(\vec{x}) = 0$ everywhere within the film, or when we Fourier transform all quantities,

$$\left[\frac{\partial^2}{\partial y^2} - Q^2 \right] \Phi(\vec{Q}, y) - 4\pi i Q_x m_x(\vec{Q}, y) - 4\pi \frac{\partial m_y(\vec{Q}, y)}{\partial y} = 0. \quad (25)$$

Here $Q^2 = Q_x^2 + Q_z^2$. Two additional relations follow from Eq. (14). These take the form

$$M_0 \frac{\partial \Phi}{\partial y}(\vec{Q}, y) + \left[H_0 + \frac{2A}{M_0} \left(Q^2 - \frac{\partial^2}{\partial y^2} \right) \right] m_y(\vec{Q}, y) = 0 \quad (26)$$

and

$$iQ_x M_0 \Phi(\vec{Q}, y) + \left[H_0 + \frac{2A}{M_0} \left(Q^2 - \frac{\partial^2}{\partial y^2} \right) \right] m_x(\vec{Q}, y) = 0. \quad (27)$$

The three statements in Eq. (25), and Eqs. (26) and (27), allow us to determine the most general form of Φ , m_x and m_y within the film. Outside the film, of course, $m_x = m_y = 0$, and also $\nabla^2 \Phi = 0$, or

$$\left[\frac{\partial^2}{\partial y^2} - Q^2 \right] \Phi(\vec{Q}, y) = 0. \quad (28)$$

We thus have fringing fields outside the film generated from a magnetic potential with the spatial variation $\exp(i\vec{Q} \cdot \vec{\rho}) \exp(-Qy)$ above the film, and $\exp(i\vec{Q} \cdot \vec{\rho}) \exp(Qy)$ below the film.

Once we find the most general solution of the magnetic potential and \vec{m} inside the film, we must match these to the magnetic field outside the film, through appropriate boundary conditions. Four boundary conditions are stated already in Eq. (3). In addition, we must insure continuity of tangential components of \vec{h} , and the normal component of \vec{B} across the actual surface of the film. It is well known that conservation of tangential \vec{h} is assured if the magnetic potentials inside and outside the film are continuous. The magnetic potentials should be matched across the actual rough surfaces. But Φ is nonzero only by virtue of the roughness. If we are interested only in the contribution to Φ first order in $\xi^>$ and $\xi^<$, it suffices to match the magnetic potentials inside and outside the film at the nominal surfaces $y = \pm D/2$.

The requirement that normal components of \vec{b} be conserved requires a bit of discussion. Consider for the moment the upper surface, and let \hat{n} be the unit normal, erected at a point. We have, in the coordinate system of Fig. 1

$$\hat{n} = \frac{1}{[1 + (\partial \xi^>/\partial x)^2 + (\partial \xi^>/\partial z)^2]^{1/2}} \left[\hat{y} - \frac{\partial \xi^>}{\partial x} \hat{x} - \frac{\partial \xi^>}{\partial z} \hat{z} \right] \approx \hat{y} - \frac{\partial \xi^>}{\partial x} \hat{x} - \frac{\partial \xi^>}{\partial z} \hat{z}, \quad (29)$$

where the last expression is to lowest order in $\xi^>$. Then just inside the film, if only first order terms are retained,

$$\hat{n} \cdot \vec{b} = -\frac{\partial \Phi}{\partial y} - 4\pi M_0 \frac{\partial \xi^>}{\partial z} + 4\pi m_y, \quad (30)$$

where the magnetic potential is evaluated at the nominal boundary $y = +D/2$. If the magnetic potential above the film is $\Phi^>$, then we conserve normal \vec{b} to first order by requiring

$$\frac{\partial \Phi}{\partial y} \Big|_{+D/2} - \frac{\partial \Phi^>}{\partial y} \Big|_{+D/2} - 4\pi m_y \Big|_{+D/2} = -4\pi M_0 \frac{\partial \xi^>}{\partial z}. \quad (31)$$

A similar statement applies at the lower surface.

We thus have a total of eight boundary conditions. Six of these, the four exchange boundary conditions, and the requirement that Φ be continuous across each surface, are homogeneous equations. In contrast, Eq. (31) and its analog on the lower surface are inhomogeneous equations. These allow us to obtain all quantities, to first order in $\xi^>$ and $\xi^<$.

We can now make one general observation, before proceeding with an explicit calculation. Suppose, say, the surface has steps of linear grooves, parallel to the applied magnetic field \vec{H}_0 and nominal magnetization \vec{M}_0 . Then $\xi^>$ and $\xi^<$ will depend only on x , so the right-hand side of Eq. (31) and its partner on the lower surface vanish. All eight boundary conditions then become homogeneous equations. In this circumstance $\Phi = m_x = m_y = 0$. The nominal magnetization \vec{M}_0 must be aligned so it has a nonzero projection along the line perpendicular to the steps or grooves for stray fields to

be generated. Since these stray fields necessarily increase the energy of the system, it follows that so far as the dipolar mechanism is concerned, the easy direction will always be parallel to edges of steps or grooves.

The structure of the analysis is now complete. We proceed by seeking solutions for m_x , m_y , and Φ within the film, through use of Eqs. (25)–(27). We seek solutions with Φ , m_x , and m_y each proportional to $\exp(-\alpha y)$. There are then three values found for α^2 . The first, α_1^2 we may call a pure exchange root:

$$\alpha_1^2 = Q^2 + \frac{M_0}{2A} H_0. \quad (32)$$

When $\alpha^2 = \alpha_1^2$, $\Phi = 0$ so no magnetic fields are generated by the spins. We have $m_y = \mp (iQ_x/\alpha)m_x$ (α is now considered as positive), for this case. Then

$$\alpha_{2,3}^2 = Q^2 + \frac{M_0}{4A} [B_0 \pm \sqrt{B_0^2 + 32\pi A Q_z^2}], \quad (33)$$

where $B_0 = H_0 + 4\pi M_0$. The most general solution for the magnetic potential in the film is then

$$\Phi(\vec{Q}, y) = \sum_{i=1}^3 [\Phi_i^{(-)} e^{-\alpha_i y} + \Phi_i^{(+)} e^{+\alpha_i y}], \quad (34)$$

and expressions for m_x and m_y follow from Eqs. (26) and (27). Above the film, we have $\Phi(\vec{Q}, y) = \Phi^> \exp(-Qy)$, and below we have $\Phi(\vec{Q}, y) = \Phi^< \exp(Qy)$. The eight constants $\Phi^>$, $\Phi^<$, $\Phi_i^{(+)}$, and $\Phi_i^{(-)}$ follow from submitting the solution just described to the boundary conditions, which we see are in the form of eight inhomogeneous equations.

We inquire into the role of the exchange in what follows. The limit $A \rightarrow 0$ describes the limit where the exchange is ignored, and only Zeeman and dipolar energies enter. As $A \rightarrow 0$, the roots α_1^2 and α_2^2 both approach infinity, and their contribution becomes vanishingly small. Then

$$\lim_{A \rightarrow 0} \alpha_3^2 = \frac{H_0}{B_0} Q_z^2 + Q_x^2. \quad (35)$$

The ‘‘dipole only’’ problem may be addressed by setting α_1 and α_2 aside, including only the terms $\exp(\pm \alpha_3 y)$ in the analysis, and employing only the boundary conditions which describe the conservation of tangential \vec{h} and normal \vec{b} .

We conclude by arranging some results above in a form where various limiting behaviors may be perceived more readily. In the ferromagnet, a fundamental length is L_N , the width of a domain wall of Néel character. In zero external magnetic field, in our notation, $L_N = (A/4\pi M_0^2)^{1/2}$. We introduce the wave vector $Q_N = 1/L_N = (4\pi M_0^2/A)^{1/2}$. When we are considering spatial modulations whose length scale is very long compared to L_N , we expect exchange to be quite unimportant in describing the spatial modulation in the magnetization, and the ‘‘dipole only’’ theory should suffice. We are then in the regime where the important wave vectors Q are small compared to Q_N . We shall see, however, that this expectation is only correct when the applied field is not too weak. Conversely, when we examine the response to wave

vectors $Q \gg Q_N$, we must incorporate exchange, to obtain an accurate description. We have, changing notation,

$$\alpha_1^2 = Q^2 + \frac{Q_N^2}{2} \left(\frac{H_0}{4\pi M_0} \right), \quad (36)$$

and

$$\alpha_{2,3}^2 = Q^2 + \frac{Q_N^2}{4} \left(\frac{B_0}{4\pi M_0} \right) \left[1 \pm \sqrt{1 + 8 \left(\frac{4\pi M_0}{B_0} \right)^2 \frac{Q_z^2}{Q_N^2}} \right]. \quad (37)$$

In the next section, we explore two simple limiting examples.

III. AN EXAMINATION OF A SIMPLE LIMITING CASE

We have carried out a series of numerical studies of step-induced anisotropy, through use of the theory developed in Sec. II. These results will be presented in Sec. IV. Before we turn to these, it is useful to explore a simple limiting case, where analytic expressions for various quantities which enter the theory may be obtained. This provides one with insight into the role of the various interactions contained within it.

Consider a semi-infinite ferromagnet, which resides in the lower half space $y < 0$. The external dc magnetic field \vec{H}_0 is parallel to the z direction, so if the surface is perfectly smooth the magnetization \vec{M}_0 is constant in direction everywhere, and parallel to \vec{H}_0 . We have $\vec{M}_0 = M_0 \hat{z}$. Now suppose $\xi^>(x, z)$ depends only on z , so if we imagine the surface contains steps, \vec{M}_0 and \vec{H}_0 are perpendicular to the step edges. Here, we confine our attention to the response of the system to a single Fourier component in the modulated surface profile, and furthermore the profile is ‘‘perpendicular’’ to the applied magnetic field, so we let $\xi^>(x, z) = \xi_0 \exp(iQz) + \text{c.c.}$ If desired, Eq. (23) applied to this circumstance may be used to synthesize an expression for ΔE for actual profiles.

One sees easily that for this case, $m_x = 0$ so only Φ and m_y are nonzero. If we seek solutions where both m_y and Φ have the spatial variation $\exp(iQz + \alpha y)$, then we find two roots for α . We refer to these as α_0 and α_x , respectively, for reasons that will be clear shortly. One has

$$\alpha_0^2 = Q^2 + \frac{M_0}{4A} [B_0 - \sqrt{B_0^2 + 32\pi A Q^2}] \quad (38)$$

and

$$\alpha_x^2 = Q^2 + \frac{M_0}{4A} [B_0 + \sqrt{B_0^2 + 32\pi A Q^2}]. \quad (39)$$

Various limiting behaviors of α_0 and α_x are of interest. First, suppose we ignore the influence of exchange, and we construct a theory where only Zeeman and dipolar energies enter. We may do this by taking the limit $A \rightarrow 0$ in all quantities. When we do this, as $A \rightarrow 0$, $\alpha_x^2 \rightarrow M_0 B_0 / 2A \rightarrow \infty$. We shall see below that in this limit, the root α_x vanishes from the problem. This is thus an ‘‘exchange root,’’ that enters the analysis by virtue of the presence of exchange. Only the ‘‘dipole root’’ α_0 remains. One has

$$\lim_{A \rightarrow 0} \alpha_0 = \left(\frac{H_0}{B_0} \right)^{1/2} Q, \quad (40)$$

a special case of Eq. (35). Here we have $Q_x = 0$, $Q_z = Q$. Notice that in zero external magnetic field, $H_0 \rightarrow 0$, in fact α_0 vanishes. If we ignore exchange, and retain only the dipolar and Zeeman energies, then in weak applied magnetic fields, the disturbance produced by modulating the surface profile penetrates very deep into the material.

However, when exchange is present, as $H_0 \rightarrow 0$, in fact α_0 remains quite well behaved and finite. One has

$$\lim_{H_0 \rightarrow 0} \alpha_0^2 = \frac{\pi M_0^2}{A} \left[1 + \frac{A Q^2}{\pi M_0^2} - \left(1 + \frac{2A Q^2}{\pi M_0^2} \right)^{1/2} \right]. \quad (41)$$

Thus, in weak applied magnetic fields, exchange enters critically in the discussion of the response of the system to modulations in the surface profile.

Now suppose we consider the limit $Q \rightarrow \infty$, or in the language used at the end of Sec. II, the regime $Q \gg Q_N$. One sees easily that

$$\lim_{Q \rightarrow \infty} \alpha_0 = \lim_{Q \rightarrow \infty} \alpha_x = Q. \quad (42)$$

We shall see implications of these limiting behaviors shortly.

It is a straightforward matter to find expressions for Φ and m_y , regarding each as superpositions of $\exp(\alpha_0 y)$ and $\exp(\alpha_x y)$, in the substrate. We have

$$m_y(y, z) = m_y(Q, y) e^{iQz} + \text{c.c.}, \quad (43)$$

and similarly for $\Phi(y, z)$. One finds, for $y < 0$,

$$m_y(Q, y) = i M_0 \xi_0 \left(\frac{\alpha_0 - Q}{\alpha_0 + \alpha_x - Q} \right) \left(\frac{\alpha_x - Q}{\alpha_x - \alpha_0} \right) \times (\alpha_x e^{\alpha_0 y} - \alpha_0 e^{\alpha_x y}), \quad (44)$$

and if we refer to the potential in the medium as $\Phi^<(Q, y)$, then

$$\Phi^<(Q, y) = \frac{4 \pi i M_0 \xi_0 \alpha_0 \alpha_x}{(\alpha_0 - \alpha_x)(\alpha_0 + \alpha_x - Q)} \times \left(\left[\frac{\alpha_x - Q}{\alpha_0 + Q} \right] e^{\alpha_0 y} - \left[\frac{\alpha_0 - Q}{\alpha_x + Q} \right] e^{\alpha_x y} \right). \quad (45)$$

Outside the material, in the region $y > 0$,

$$\Phi^>(Q, y) = - \frac{i 4 \pi M_0 (\alpha_0 + \alpha_x) \alpha_0 \alpha_x \xi_0}{(\alpha_0 + \alpha_x - Q)(\alpha_0 + Q)(\alpha_x + Q)} \exp(-Qy). \quad (46)$$

Notice that in all the expressions above, if we ignore exchange by taking the limit $A \rightarrow 0$, α_x indeed drops out of all the expressions, and only the ‘‘dipole root’’ remains.

Finally, the energy change per unit area $\Delta E/A$ produced by modulating the surface profile is

$$\frac{\Delta E}{A} = \frac{4 \pi M_0^2 Q |\xi_0|^2 \alpha_0 \alpha_x (\alpha_0 + \alpha_x)}{(\alpha_0 + Q)(\alpha_x + Q)(\alpha_0 + \alpha_x - Q)}. \quad (47)$$

Suppose now that we keep the magnetization pinned rigidly in place, in the presence of the modulated surface profile.

That is, we overlook the fact that the magnetization direction varies in the substrate, after the surface profile is modulated. Then stray magnetic fields are generated only by the magnetic charges on the surface. If we refer to the magnetic potential in this picture as $\Phi^{(0)}(y, z)$, and the energy change as $\Delta E^{(0)}$, then for all values of y we have

$$\Phi^{(0)}(y, z) = -i 2 \pi M_0 \xi_0 \exp(-Q|y|) \exp(iQz), \quad (48)$$

and one finds

$$\frac{\Delta E^{(0)}}{A} = 2 \pi M_0^2 Q |\xi_0|^2. \quad (49)$$

Of interest is the ratio $\Delta E/\Delta E^{(0)}$; this provides us with the error we make if we assume simply that the magnetization is fixed rigidly, with fields generated by the surface magnetic poles. We have

$$\frac{\Delta E}{\Delta E^{(0)}} = \frac{2 \alpha_0 \alpha_x (\alpha_0 + \alpha_x)}{(\alpha_0 + Q)(\alpha_x + Q)(\alpha_0 + \alpha_x - Q)}. \quad (50)$$

On physical grounds, it is the case always that $\Delta E/\Delta E^{(0)} < 1$. That is, the ‘‘rigid magnetization’’ picture always overestimates the step-induced anisotropy. This follows because ΔE is the change in energy produced by a magnetization distribution that minimizes the total energy of the system. Hence, $\Delta E < \Delta E^{(0)}$ always. Let us suppose that we ignore the influence of the exchange by allowing A to vanish. Then as we have seen, $\alpha_x \rightarrow \infty$, and if we refer to the energy change in this case as $\Delta E^{(DIP)}$, we have

$$\frac{\Delta E^{(DIP)}}{\Delta E^{(0)}} = \frac{2 \alpha_0}{\alpha_0 + Q}, \quad (51)$$

or with $\alpha_0 = (H_0/B_0)^{1/2} Q$ in this limit, we have

$$\frac{\Delta E^{(DIP)}}{\Delta E^{(0)}} = \frac{2 H_0^{1/2}}{B_0^{1/2} + H_0^{1/2}}. \quad (52)$$

In the weak-field regime, $H_0 \ll 4 \pi M_0$, we have a strongly field-dependent step-induced anisotropy energy. When $H_0 \gg 4 \pi M_0$, $\Delta E^{(DIP)}$ does approach the rigid magnetization limit.

Now we explore the full theory, with exchange included. We then encounter a characteristic length scale, the width L_N of the Néel wall, discussion in Sec. II. We have the characteristic wave vector $Q_N = (4 \pi M_0^2/A)^{1/2}$. When $Q \gg Q_N$, we are considering a surface with features on the length scale small compared to L_N , and when $Q \ll Q_N$, the length scale is very long compared to Q_N .

When $Q \gg Q_N$, we have seen above that $\alpha_0 \approx \alpha_x \approx Q$. In this regime, we find

$$\frac{\Delta E}{\Delta E^{(0)}} \approx 1. \quad (53)$$

As one would expect, the magnetization cannot follow features on such a small length scale, and the rigid magnetization picture works well.

The regime $Q \ll Q_N$ is a bit more complex. In this limit

$$\alpha_x \approx \frac{Q_N}{\sqrt{2}} \left(\frac{B_0}{4\pi M_0} \right)^{1/2}, \quad (54)$$

while α_0 is well approximated by

$$\alpha_0 = Q \left[\frac{H_0}{B_0} + 2 \left(\frac{4\pi M_0}{B_0} \right)^2 \frac{Q^2}{Q_N^2} \right]^{1/2}. \quad (55)$$

Clearly $\alpha_x \gg \alpha_0$, so to excellent approximation

$$\frac{\Delta E}{\Delta E^{(0)}} \approx \frac{2\alpha_0}{\alpha_0 + Q}, \quad (56)$$

as in Eq. (51). If the applied external field H_0 is very weak, we find an additional length scale long compared to L_N enters the problem. This is $L_c = (B_0/H_0)^{1/2} L_N$. Associated with this is the wave vector $Q_c = Q_N (H_0/B_0)^{1/2}$. Thus, α_0 can be written as

$$\alpha_0 = Q \left[\frac{Q_c^2}{Q_N^2} + 2 \left(\frac{4\pi M_0}{B_0} \right)^2 \frac{Q^2}{Q_N^2} \right]^{1/2}. \quad (57)$$

When $H_0 \ll 4\pi M_0$ or $Q_c \ll Q_N$, we have two regimes:

(i) $Q_c \ll Q \ll Q_N$: Then $\alpha_0 \approx \sqrt{2} Q^2 / Q_N$, and we have

$$\frac{\Delta E}{\Delta E^{(0)}} \approx 2 \frac{\sqrt{2} Q}{Q_N} \gg 2 \left(\frac{H_0}{B_0} \right)^{1/2} = 2 \frac{Q_c}{Q_N}. \quad (58)$$

While one's first thought is that for length scales long compared to L_N , exchange effects can be set aside, and the "dipole only" theory should be appropriate, we see exchange still enters importantly. The theory with exchange ignored underestimates the roughness-induced anisotropy substantially.

(ii) $0 \ll Q \ll Q_c \ll Q_N$: Here $\alpha_0 \approx (H_0/B_0)^{1/2} Q$, the "dipole only" result, and one may safely ignore the influence of exchange.

In any real material, of course, anisotropy will be present. If the external field H_0 is applied parallel to the easy axis, then one may include anisotropy by replacing H_0 by $(H_0 + H_a)$, with H_a the strength of the effective anisotropy field. For Fe, as an example, $H_a \approx 550$ G, while $4\pi M_0 = 21$ kG. Thus this material, in zero external magnetic field, can be characterized by the ratio $H_0^{(\text{eff})}/4\pi M_0 \approx 0.02$. The weak-field limit just discussed thus applies to Fe in zero external magnetic field, with anisotropy treated in this manner.

IV. NUMERICAL STUDIES OF DIPOLAR ANISOTROPY INDUCED BY UNIDIRECTIONAL SURFACE PROFILE MODULATION

We have carried out numerical studies of the dipolar anisotropy induced by unidirectional modulation of the surface profile, with emphasis on the case where one has a film deposited on a stepped surface. We have ultrathin (few atomic layer) films in mind for these studies, because of the recent experimental interest in such films grown on substrates with steps. All of our calculations use parameters characteristic of Fe, for which $M_0 = 1.7 \times 10^3$ G, and $A = 2.1 \times 10^{-6}$ erg/cm.

For a stepped surface, and the case where the step edges

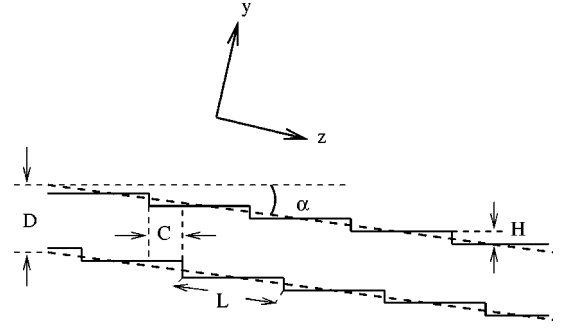


FIG. 3. Geometry of a film with stepped surfaces. The upper and lower steps are displaced by a distance C , the steps height is H , the resultant angle of "descent" (or "ascent") is $\alpha \approx H/L$, with L the period of the steps.

are perpendicular to the magnetic field, we show the geometry we have employed in Fig. 3. Unless otherwise specified, the nominal film thickness D has been chosen to be 10 \AA , the step height $H = 2 \text{ \AA}$, appropriate to monatomic steps, and the applied field as $H_0 = 0.1 \times 4\pi M_0$. We also have chosen the offset $C = 2 \text{ \AA}$, in the initial set of results to be shown below. It should be remarked that we have explored the influence of C on the anisotropy, to find its influence rather weak. If C varies from 0 to 20 \AA , for the angle $\alpha = H/L$ of one degree, the step-induced anisotropy changes by less than 10%.

The first question is the angular variation of the stepped-induced anisotropy. We have seen in Sec. II that within our perturbation theoretic treatment, the easy axis is always parallel to the step edges. Our numerical studies show $\Delta E(\theta)$ to vary quite accurately as $\cos^2(\theta)$. The deviations, for the full theory with exchange included, are in the range of 1%, or less. Thus, we have simple uniaxial anisotropy, to an excellent approximation, so far as we can see. Because of this, in what follows, we shall confine our attention to the step-induced energy change for the case where the step edges are perpendicular to \vec{H}_0 , where the magnetization is parallel to the hard direction. The reader may assume the $\cos^2 \theta$ variation applies. For this special case, it is possible to derive relatively simple expressions for the various quantities, through a suitable extension of the discussion presented in Sec. III. We summarize the expressions in the Appendix.

We first consider the variation of the step-induced anisotropy with magnetic field H_0 . For the case where the angle $\alpha \approx H/L$ is one degree, we show the field dependence in Fig. 4. We show this calculated for the full theory with exchange included, and for the case where we ignore exchange and include only the Zeeman and dipolar energies. In the latter case, we see a very strong dependence on H_0 similar qualitatively to that contained in Eq. (52) for the semi-infinite case. This very strong field dependence is suppressed when exchange is included; the field dependence is then very weak.

In Fig. 5, we show the dependence of the anisotropy on the angle α . For very small angles, we have a linear variation, and with increasing angle the strength of the anisotropy increases somewhat more slowly than linearly. Something close to linear behavior has been observed experimentally for a Co film on a curved Cu (001) substrate. In that case the easy axis is also parallel to the step edges. The authors of

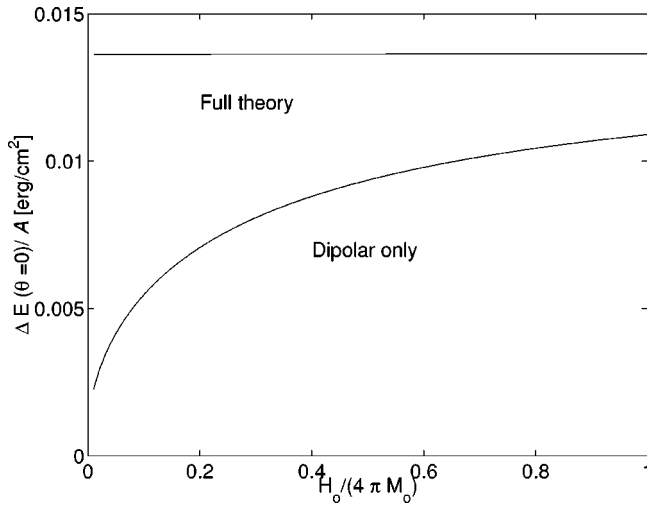


FIG. 4. Change of magnetic energy per surface area as a function of applied field, for a geometry with stepped surfaces. The energy change is plotted for the applied field perpendicular to the steps and including (full theory) and excluding the exchange term (dipolar only). In this case $H=C=2 \text{ \AA}$, $D=10 \text{ \AA}$, and $\alpha=1^\circ$. When the exchange term is included, the exchange constant corresponds to Fe.

Ref. 8 propose a mechanism different than that exposed here, in their discussion of the anisotropy.

It is the case, however, that the magnitude of the anisotropy is in the range of that found experimentally, for the ultrathin films studied. We find, for α in the range of a few degrees, that $\Delta E \approx 0.02 - 0.04 \text{ ergs/cm}^2$. If we express ΔE in terms of an effective magnetic field acting on the magnetization in the film, then $\Delta E = M_0 D H^{(\text{eff})}$, for a film of thickness D . For Fe, $M_0 \approx 1.7 \times 10^3 \text{ G}$, so if $D = 10 \text{ \AA}$ and $\Delta E = 0.04 \text{ ergs/cm}^2$, then $H^{(\text{eff})} \approx 240 \text{ G}$, in the range found experimentally for stepped-induced anisotropy in ultrathin films. Thus, while other mechanisms surely contribute as

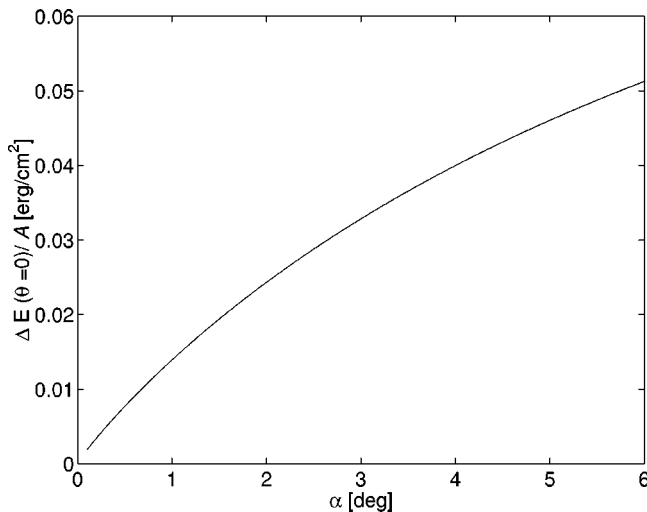


FIG. 5. Change of magnetic energy per surface area as a function of angle of "descent" (or "ascent"), for a geometry with stepped surfaces. The energy change is plotted for the applied field perpendicular to the steps and including an exchange term corresponding to Fe. In this case $H=C=2 \text{ \AA}$, $D=10 \text{ \AA}$, and $H_0=0.1 \times 4\pi M_0$.

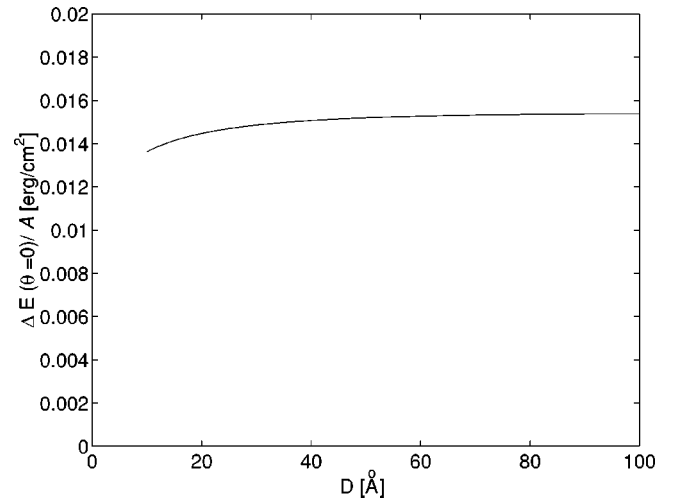


FIG. 6. Change of magnetic energy per surface area as a function of film thickness, for a geometry with stepped surfaces. The energy change is plotted for the applied field perpendicular to the steps and including an exchange term corresponding to Fe. In this case $H=C=2 \text{ \AA}$, $\alpha=1^\circ$, and $H_0=0.1 \times 4\pi M_0$.

well, the contribution explored here should play an important role in real materials, possibly for the Co film on Cu (001) studied in Ref. 8.

In Fig. 6, we show the dependence of ΔE on film thickness, for thicknesses in the range from 10 to 100 \AA . Throughout this range, we see that ΔE exhibits a very weak dependence on D . It is common to divide the strength of anisotropies measured in ultrathin films by D , and then plot the result as a function of D itself. Volume anisotropies are independent of D , while surface anisotropies provide a contribution inversely proportional to D , when the data is displayed in this manner. From Fig. 6, we see that despite the long-range nature of the dipolar fields, the step-induced anisotropy behaves very much like a surface anisotropy.

We conclude with information on the spatial distribution and magnitude of both the stray fields and magnetization, for a particular profile illustrated in Fig. 7. We have a film whose nominal thickness is 40 \AA , with upper surface at $y=20 \text{ \AA}$, and lower surface at $y=-20 \text{ \AA}$. Steps are located at $z=40 \text{ \AA}$ and $z=60 \text{ \AA}$. The terrace length is $L=100 \text{ \AA}$, and the step height has been adjusted so that $\alpha=H/L=1^\circ$.

In Fig. 8, we show the variation of h_z with z evaluated at the center plane ($y=0 \text{ \AA}$) of films of thickness $D=40 \text{ \AA}$ corresponding to case (a) and $D=10 \text{ \AA}$ to case (b). We see that in the center of the film the field can be as large as a half of $4\pi M_0$ for the thinner film (recall that for Fe, $4\pi M_0 = 21 \text{ kG}$). However, if one evaluates h_z close to the surfaces of the films, one sees that near the steps (located at $z=40 \text{ \AA}$ and $z=60 \text{ \AA}$) h_z assumes very large values indeed, so within a few Angstroms of a step h_z assumes values large compared to $4\pi M_0$.

We show the variation with the coordinate y of the component h_y in Fig. 9. Once again, near the steps, very large stray fields are generated. One can perceive one aspect of the field distribution, illustrated more clearly below, from these curves. The step on the upper surface behaves as a positive line charge, out of which magnetic-field lines diverge. In contrast, the step on the lower surface acts as a negative

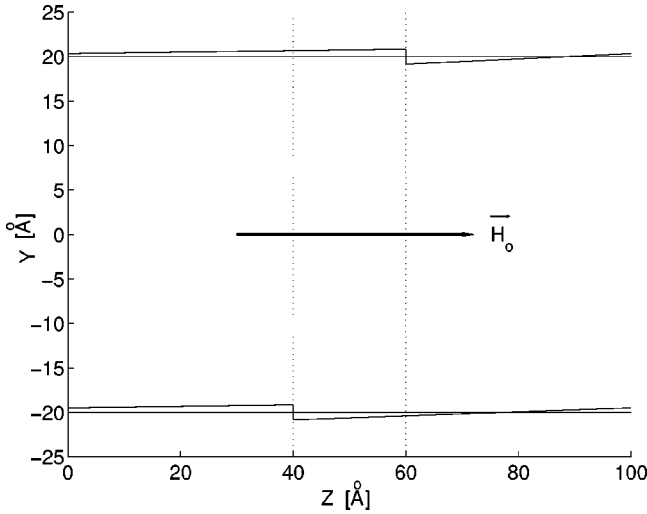


FIG. 7. Geometry of a stepped surface of period $L = 100 \text{ \AA}$, with steps separated by a distance $C = 20 \text{ \AA}$, and angle of ‘‘descent’’ (or ‘‘ascent’’) $\alpha = 1^\circ$. The field \vec{H}_0 is applied in the film plane ($H_0 = 0.1 \times 4\pi M_0$), and the film thickness is 40 \AA . This geometry corresponds to the plots of Figs. 8–12. The exchange constant for those plots corresponds to that of Fe.

magnetic line charge. Field lines diverge outward from the former, and inward from the latter. The two steps thus act as a magnetic dipole in two dimensions, i.e., we have a positive line charge in near proximity to a negative line charge.

In Fig. 10, we show the variation of m_y throughout the film, within the framework of a calculation which sets the strength of the exchange stiffness A to zero. We see that the perturbation of the magnetization is confined to the near vicinity of the steps. However, inclusion of exchange alters this picture qualitatively, as we see from the full calculation with exchange included, presented in Fig. 11. The perturbation in the magnetization produced by the steps now extends throughout the film. For any choice of the coordinate y , we see a nearly sinusoidal spatial variation in the magnetization.

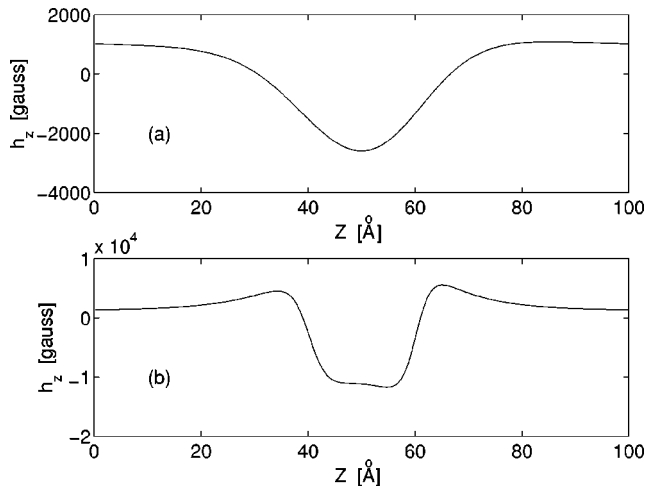


FIG. 8. Plots of the z component of the stray field due to the roughness of a geometry with stepped surfaces. This component of the field is plotted along a line that goes through the middle plane of the film ($Y = 0 \text{ \AA}$), for films of thicknesses $D = 40 \text{ \AA}$ for case (a) and $D = 10 \text{ \AA}$ for case (b).

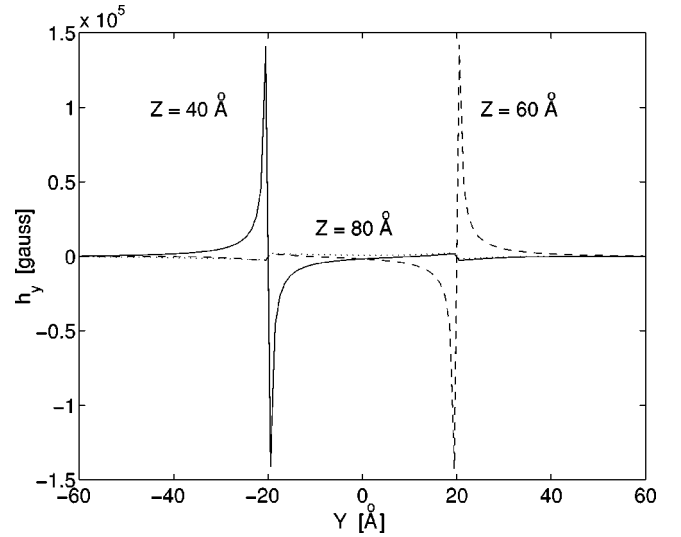


FIG. 9. Plot of the y component of the stray field due to the roughness of a geometry with stepped surfaces. This component of the field is plotted along vertical lines that pass close to the lower step at $Z = 40 \text{ \AA}$ and to the upper step at $Z = 60 \text{ \AA}$, and along a vertical line separated from the steps (at $Z = 80 \text{ \AA}$).

If one realizes that $\hat{n} \cdot \vec{M}$ acts as an effective magnetic surface charge density, and notes that the outward normal \hat{n} is oppositely directed on the upper and lower surface, one sees the origin of the magnetic dipole discussed in the previous paragraphs. The piece $\hat{n} \cdot \vec{M}_0$ evaluated on the step edges is the dominant source of surface charge.

We conclude in Fig. 12 with a figure which shows the spatial variation of the magnetic-field lines, along with equipotential surfaces for the magnetic potential. We see field lines diverging from the step on the upper surface, and converging into that on the lower surface.

V. FINAL REMARKS

Within a continuum theory, we have presented a description of the influence of surface roughness on the distribution

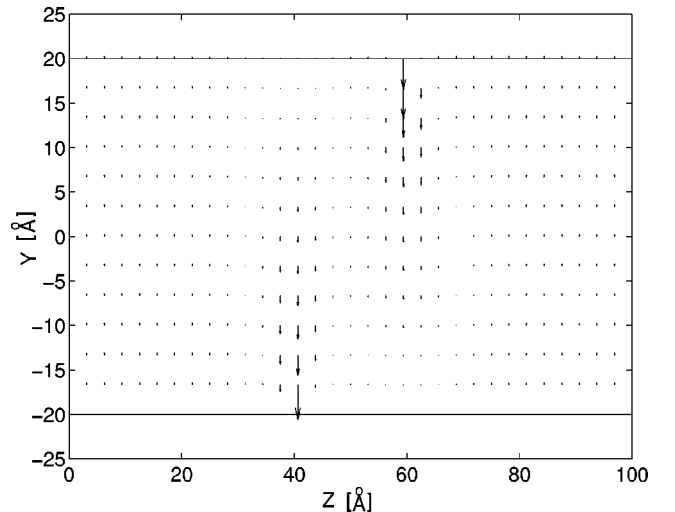


FIG. 10. Schematics of the y component of the magnetization induced by the roughness of a geometry with stepped surfaces. A relative magnitude is plotted at different points of the film. This case corresponds to the dipolar only theory (exchange excluded).

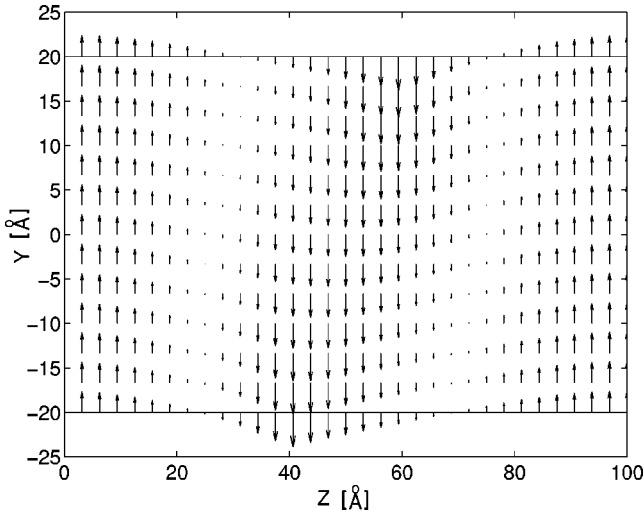


FIG. 11. Schematics of the y component of the magnetization induced by the roughness of a geometry with stepped surfaces. A relative magnitude is plotted at different points of the film. This case corresponds to the full theory (exchange included).

of magnetization within a ferromagnetic film. Stray magnetic fields are generated, and the magnetic energy per unit area is increased by these effects. When the roughness has a unidirectional character, as is the case for a film grown on a stepped surface, the increase in the magnetic energy per unit area depends on the direction between the nominal magnetization, and the step edges. We thus have a mechanism for step-induced anisotropy.

Within our perturbation theoretic description of the dipolar contribution to the anisotropy energy, the easy axis will always be parallel to the step edges. Its strength varies linearly with the vicinal angle $\alpha = H/L$ for small α , according to our numerical studies, and increases more slowly for larger values. For the model films explored, we find anisotropy energies fall in the range of those found experimentally. Thus, the mechanism explored here should be an important source of step-induced anisotropy. However, as noted in Sec.

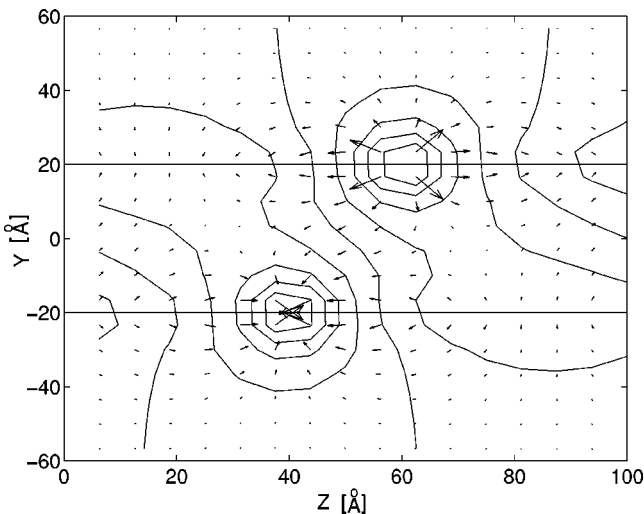


FIG. 12. Graphic representation of the stray fields and magnetic potential induced by the roughness of a geometry with stepped surfaces. Lines represent equipotentials, and arrows the direction and relative magnitude of the (y, z) components of the stray fields.

I, other mechanisms surely contribute as well. Experiments show this is the case as well, since for some samples one sees a quadratic variation of the step-induced anisotropy with α . Also, the easy axis may be normal to, and not parallel to the step edges in some cases. Further study is clearly required to establish the conditions under which a given mechanism may dominate.

The theory presented here should enable one to address other influences of interface roughness on the properties of ultrathin ferromagnetic films, and with suitable extensions, in the properties of magnetic multilayers.

ACKNOWLEDGMENTS

This research was completed with support from the Army Research Office, under Contract No. CS0001028. R.A. was given partial financial support by the Organization of American States.

APPENDIX

Here we summarize the expressions for the perturbation of the magnetization, magnetic potential, and energy of a thin ferromagnetic film whose upper and lower surfaces have arbitrary unidirectional roughnesses. It is also assumed that the applied field $\vec{H}_0 = H_0 \hat{z}$ (in the plane of the film) is perpendicular to the roughness features.

The roughnesses of the upper and lower surfaces of the film are written as

$$\xi^{u,d}(z) = \sum_{Q_n} \xi_{Q_n}^{u,d} e^{iQ_n z} \quad (\text{A1})$$

with $Q_n = 2\pi n/\mathcal{L}$, $n = -\infty, \dots, \infty$, and \mathcal{L} a quantization length. For simplicity we will concentrate only on one wavelength, i.e., we assume

$$\xi^{u,d}(z) = \xi_Q^{u,d} e^{iQz} + \text{c.c.} \quad (\text{A2})$$

with $\xi_Q^{u,d} \equiv |\xi_Q^{u,d}| e^{i\psi_Q^{u,d}}$ [the results for an arbitrary roughness, as that of Eq. (A1), follow by simple superposition]. Due to the symmetry of this geometry, $m_x^Q(y, z) = 0$. The following forms of $m_y^Q(y, z)$ and $\phi_Q(y, z)$, valid inside the film, solve to first order the equilibrium equation $\vec{M} \times \vec{H}_{\text{eff}} = 0$ and the Maxwell equation $\vec{\nabla} \cdot \vec{B} = 0$:

$$\begin{aligned} m_y^Q(y, z) = & [A^x (\alpha_x^2 - Q^2) \cosh(\alpha_x y) + A^0 (\alpha_0^2 - Q^2) \cosh(\alpha_0 y) \\ & + S^x (\alpha_x^2 - Q^2) \sinh(\alpha_x y) \\ & + S^0 (\alpha_0^2 - Q^2) \sinh(\alpha_0 y)] e^{iQz} + \text{c.c.}, \end{aligned} \quad (\text{A3})$$

$$\begin{aligned} \phi_Q(y, z) = & 4\pi [A^x \alpha_x \sinh(\alpha_x y) + A^0 \alpha_0 \sinh(\alpha_0 y) \\ & + S^x \alpha_x \cosh(\alpha_x y) + S^0 \alpha_0 \cosh(\alpha_0 y)] e^{iQz} + \text{c.c.}, \end{aligned} \quad (\text{A4})$$

and outside the film, in the upper and lower regions, respectively, the potential reads as

$$\begin{aligned} \phi_Q^u(y, z) = & 4\pi[A^x \alpha_x \sinh(\alpha_x D/2) + A^0 \alpha_0 \sinh(\alpha_0 D/2) \\ & + S^x \alpha_x \cosh(\alpha_x D/2) \\ & + S^0 \alpha_0 \cosh(\alpha_0 D/2)] e^{-Q(y-D/2)+iQz} + \text{c.c.}, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} \phi_Q^d(y, z) = & -4\pi[A^x \alpha_x \sinh(\alpha_x D/2) + A^0 \alpha_0 \sinh(\alpha_0 D/2) \\ & - S^x \alpha_x \cosh(\alpha_x D/2) \\ & - S^0 \alpha_0 \cosh(\alpha_0 D/2)] e^{Q(y+D/2)+iQz} + \text{c.c.} \end{aligned} \quad (\text{A6})$$

In these expressions the ‘‘decay constants’’ α_0 and α_x are the same as the exchange and dipolar decay constants of Eqs. (38) and (39), that correspond to the analogous problem on a semi-infinite medium. The four constants A^x , A^0 , S^x , and S^0 are obtained by applying the boundary conditions of null normal derivatives of the magnetization at the upper and lower surfaces, and both \vec{H}_Q^{tang} (or equivalently Φ_Q) and $\vec{B}_Q^{\text{normal}}$ continuous at the upper and lower surfaces of the film. These constants become

$$\begin{aligned} A_x = \frac{iM_0}{2F_Q} d_0(\xi_Q^u + \xi_Q^d), \quad A_0 = -\frac{iM_0}{2F_Q} d_x(\xi_Q^u + \xi_Q^d), \\ S_x = \frac{iM_0}{2B_Q} a_0(\xi_Q^u - \xi_Q^d), \quad S_0 = -\frac{iM_0}{2B_Q} a_x(\xi_Q^u - \xi_Q^d) \end{aligned} \quad (\text{A7})$$

with

$$\begin{aligned} a_0 &\equiv \alpha_0(\alpha_0^2 - Q^2) \cosh(\alpha_0 D/2), \\ a_x &\equiv \alpha_x(\alpha_x^2 - Q^2) \cosh(\alpha_x D/2), \\ d_0 &\equiv \alpha_0(\alpha_0^2 - Q^2) \sinh(\alpha_0 D/2), \\ d_x &\equiv \alpha_x(\alpha_x^2 - Q^2) \sinh(\alpha_x D/2), \end{aligned} \quad (\text{A8})$$

and

$$\begin{aligned} B_Q &\equiv \alpha_0 \alpha_x (\alpha_x^2 - \alpha_0^2) \cosh(\alpha_x D/2) \cosh(\alpha_0 D/2) \\ &+ \alpha_x (\alpha_x^2 - Q^2) Q \cosh(\alpha_x D/2) \sinh(\alpha_0 D/2) \\ &- \alpha_0 (\alpha_0^2 - Q^2) Q \cosh(\alpha_0 D/2) \sinh(\alpha_x D/2), \\ F_Q &\equiv \alpha_0 \alpha_x (\alpha_x^2 - \alpha_0^2) \sinh(\alpha_x D/2) \sinh(\alpha_0 D/2) \\ &+ \alpha_x (\alpha_x^2 - Q^2) Q \sinh(\alpha_x D/2) \cosh(\alpha_0 D/2) \\ &- \alpha_0 (\alpha_0^2 - Q^2) Q \cosh(\alpha_x D/2) \sinh(\alpha_0 D/2). \end{aligned} \quad (\text{A9})$$

The change in energy per unit surface area due to this single Fourier component (Q) follows from use of Eq. (23):

$$\begin{aligned} \frac{\Delta E_Q}{A} = & 2\pi M_0^2 Q \alpha_0 \alpha_x (\alpha_x^2 - \alpha_0^2) \left\{ \frac{1}{F_Q} [|\xi_Q^u|^2 + |\xi_Q^d|^2] \right. \\ & + 2|\xi_Q^u||\xi_Q^d| \cos(\psi_Q^u - \psi_Q^d) \sinh(\alpha_x D/2) \sinh(\alpha_0 D/2) \\ & + \frac{1}{B_Q} [|\xi_Q^u|^2 + |\xi_Q^d|^2 - 2|\xi_Q^u||\xi_Q^d| \cos(\psi_Q^u - \psi_Q^d)] \\ & \left. \times \cosh(\alpha_x D/2) \cosh(\alpha_0 D/2) \right\}. \end{aligned} \quad (\text{A10})$$

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