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Letter to the Editor

Evaluation of the magnetic dipolar fields from layered systems on atomic scale

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Abstract

Exact analytical expressions for the magnetic dipolar fields produced by a plane square lattice with localized magnetic moments are derived. Basing on these expressions surface roughness of a magnetic thin film is considered. Influence of the dipolar fields on the surface anisotropy and hyperfine fields is discussed.

1. Introduction

Recent advances in magnetism of thin films [1] demonstrate the possibility to investigate experimentally local magnetic properties such as hyperfine fields of monoatomic layers [2], surface anisotropies [3], isolated domain walls [4], magnetic moments of single atoms [5], coupling between thin magnetic films [6] and others. However, a detailed theoretical analysis of these local characteristics of thin magnetic films requires taking into account many factors which make this analysis extremely complicated. A typical example of such a situation are the calculations of magnetic moments and hyperfine fields in the vicinity of an interface [7]. They require many hours of computer time even for an ideal case, i.e. in the absence of roughness, interdiffusion, defects and impurities. In this situation it may be important to know physical quantities which influence these local characteristics and can be calculated exactly, i.e. without any approximations. One of such quantities is a dipolar field, created by magnetic layers and acting on surrounding atoms of a thin film.

In the framework of a continuous approach an infinite two-dimensional ferromagnetic layer with in-plain magnetization does not produce a magnetic field outside itself. Only the presence of the atomic structure of the matter and the localization of magnetic spins results in a magnetic field outside the layer [8]. Using computer calculations, it has been shown [9] that for a square lattice at a given distance from the layer the dipolar field is spatially periodic and decays exponentially with distance from the plane. However, since the dipolar interaction is of long range, a summation of dipolar fields is a very complicated procedure, especially if one tries to take into account surface roughness. Therefore, it is very useful to derive exact analytical expressions, which will provide physicists with an clear understanding of the result being obtained and allow them to use these expressions for the analysis of the influence of dipolar fields on the local magnetic properties of layered systems.

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2. Magnetic dipolar field of a plane square lattice

The magnetic dipolar field $\boldsymbol{H}$ created by a magnetic moment $\boldsymbol{\mu}$ at a distance $\boldsymbol{r}$ can be written as follows:

$$\boldsymbol{H}(\boldsymbol{r}) = -\left\{\frac{\boldsymbol{\mu}}{r^3} - 3\frac{(\boldsymbol{\mu}\boldsymbol{r})\boldsymbol{r}}{r^5}\right\}. \tag{1}$$

In analogy with the respective electrostatic problem it is convenient to introduce a scalar potential

$$\Phi(\boldsymbol{r}) = \frac{(\boldsymbol{\mu}\boldsymbol{r})}{r^3}, \tag{2}$$

correlated with the field as follows:

$$\boldsymbol{H} = -\boldsymbol{\nabla}\Phi. \tag{3}$$

Let us consider a two-dimensional infinite ferromagnetic layer magnetized in plane, i.e. a plane consisting of a square lattice of magnetic moments $\boldsymbol{\mu}$ oriented in x-direction as it is shown in Fig. 1. It is clear from the figure that

$$\boldsymbol{R} = \{x, y, z\}, \qquad \boldsymbol{\rho} = \{na, ma, 0\}, \qquad \boldsymbol{r} = \boldsymbol{R} - \boldsymbol{\rho} = \{x - na, y - ma, z\}, \tag{4}$$

here $\boldsymbol{R}$ determines a point where the dipolar field is calculated, $\boldsymbol{\rho}$ is a radius-vector of a magnetic moment within the plane, a is lattice parameter, n, m are integers. Therefore, the potential Φ produced by a square lattice of magnetic moments is given by the following expression:

$$\Phi(x, y, z) = \sum_{n,m=-\infty}^{\infty} \frac{\mu(x - na)}{\left[(x - na)^2 + (y - ma)^2 + z^2\right]^{3/2}}. \tag{5}$$

Because of slow convergence, the direct summation in formula (5) is extremely time-consuming. It is significantly more useful to transform (5) into a series of exponential terms. For that it is convenient to apply Poisson's formula, which reduces the sum of functions $f(x)$ at points na to the sum of their Fourier components:

$$\sum_{n=-\infty}^{\infty} f(na) = \frac{1}{a} \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) \exp\left(-\mathrm{i}k\frac{2\pi}{a}x\right) \mathrm{d}x. \tag{6}$$

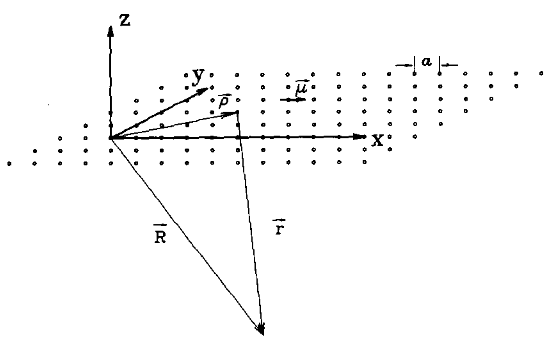

Fig. 1. Plane square lattice of magnetic moments. $\boldsymbol{R}$ denotes the radius-vector of a point where the dipolar field is calculated.

Using (5) and (6) after simple transformation one obtains

$$\Phi(x, y, z) = \frac{\mu}{a^2} \sum_{k,l=-\infty}^{\infty} \exp\left(-ik\frac{2\pi}{a}x\right) \exp\left(-il\frac{2\pi}{a}y\right)$$
$$\times \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{x_1}{\left(x_1^2+y_1^2+z^2\right)^{3/2}} \exp\left(ik\frac{2\pi}{a}x_1\right) \exp\left(il\frac{2\pi}{a}y_1\right) \mathrm{d}x_1\, \mathrm{d}y_1. \tag{7}$$

The double integral in (7) can be calculated analytically and it is equal to

$$2\pi \mathrm{i} \frac{k}{\sqrt{k^2+l^2}} \exp\left(-\frac{2\pi}{a}\sqrt{k^2+l^2}\,|z|\right). \tag{8}$$

After a straightforward transformation we finally have

$$\Phi(x, y, z) = \frac{4\pi\mu}{a^2}\left\{ \sum_{k=1}^{\infty} \sin\left(\frac{2\pi}{a}kx\right) \exp\left(-\frac{2\pi}{a}k|z|\right)\right.$$
$$\left. +2 \sum_{k,l=1}^{\infty} \frac{k}{\sqrt{k^2+l^2}} \sin\left(\frac{2\pi}{a}kx\right) \cos\left(\frac{2\pi}{a}ly\right) \exp\left(-\frac{2\pi}{a}\sqrt{k^2+l^2}\,|z|\right)\right\}. \tag{9}$$

The projections of the magnetic dipolar field $\boldsymbol{H}$ can be easily derived from Eq. (9) by differentiation in accordance with (3):

$$H_x = -\frac{8\pi^2\mu}{a^3}\left\{ \sum_{k=1}^{\infty} k \cos\left(\frac{2\pi}{a}kx\right) \exp\left(-\frac{2\pi}{a}k|z|\right)\right.$$
$$\left. +2 \sum_{k,l=1}^{\infty} \frac{k^2}{\sqrt{k^2+l^2}} \cos\left(\frac{2\pi}{a}kx\right) \cos\left(\frac{2\pi}{a}ly\right) \exp\left(-\frac{2\pi}{a}\sqrt{k^2+l^2}\,|z|\right)\right\}, \tag{10a}$$

$$H_y = \frac{16\pi^2\mu}{a^3}\left\{ \sum_{k,l=1}^{\infty} \frac{kl}{\sqrt{k^2+l^2}} \sin\left(\frac{2\pi}{a}kx\right) \sin\left(\frac{2\pi}{a}ly\right) \exp\left(-\frac{2\pi}{a}\sqrt{k^2+l^2}\,|z|\right)\right\}, \tag{10b}$$

$$H_z = \mathrm{sign}(z)\frac{8\pi^2\mu}{a^3}\left\{ \sum_{k=1}^{\infty} k \sin\left(\frac{2\pi}{a}kx\right) \exp\left(-\frac{2\pi}{a}k|z|\right)\right.$$
$$\left. +2 \sum_{k,l=1}^{\infty} k \sin\left(\frac{2\pi}{a}kx\right) \cos\left(\frac{2\pi}{a}ly\right) \exp\left(-\frac{2\pi}{a}\sqrt{k^2+l^2}\,|z|\right)\right\}. \tag{10c}$$

It is seen from Eq. (10) that the dipolar field is spatially periodic with the lattice constant a. Each harmonic of this periodic function falls off exponentially with the distance z from the plane. For practical calculations of the dipolar field beyond the plane ($z \gtrsim a$) it is sufficient to take into account only several first harmonics in Eq. (10).

Using a similar technique one can derive formulas for the magnetic dipolar field produced by a two-dimensional infinite ferromagnetic layer magnetized perpendicular to the plain:

$$H_x = \mathrm{sign}(z)\frac{8\pi^2\mu}{a^3}\left\{ \sum_{k=1}^{\infty} k \sin\left(\frac{2\pi}{a}kx\right) \exp\left(-\frac{2\pi}{a}k|z|\right)\right.$$
$$\left. +2 \sum_{k,l=1}^{\infty} k \sin\left(\frac{2\pi}{a}kx\right) \cos\left(\frac{2\pi}{a}ly\right) \exp\left(-\frac{2\pi}{a}\sqrt{k^2+l^2}\,|z|\right)\right\}, \tag{11a}$$

$$H_y = \text{sign}(z)\frac{8\pi^2\mu}{a^3}\left\{\sum_{l=1}^{\infty} l \sin\left(\frac{2\pi}{a}ly\right)\exp\left(-\frac{2\pi}{a}l|z|\right)\right.$$

$$\left.+2\sum_{k,l=1}^{\infty} l\cos\left(\frac{2\pi}{a}kx\right)\sin\left(\frac{2\pi}{a}ly\right)\exp\left(-\frac{2\pi}{a}\sqrt{k^2+l^2}\,|z|\right)\right\}, \tag{11b}$$

$$H_z = \frac{8\pi^2\mu}{a^3}\left\{\sum_{k=1}^{\infty} k\cos\left(\frac{2\pi}{a}kx\right)\exp\left(-\frac{2\pi}{a}k|z|\right) + \sum_{l=1}^{\infty} l\cos\left(\frac{2\pi}{a}ly\right)\exp\left(-\frac{2\pi}{a}l|z|\right)\right.$$

$$\left.+2\sum_{k,l=1}^{\infty}\sqrt{k^2+l^2}\cos\left(\frac{2\pi}{a}kx\right)\cos\left(\frac{2\pi}{a}ly\right)\exp\left(-\frac{2\pi}{a}\sqrt{k^2+l^2}\,|z|\right)\right\}. \tag{11c}$$

Basing on Eqs. (10), (11) it is easy to calculate dipolar fields produced by an infinite antiferromagnetic layer magnetized both in and perpendicular to the plane. In order to do that one should consider the plane antiferromagnetic lattice as that consisting of two square sublattices with opposite orientation of the magnetic moments and add the contributions from both sublattices. The derived expressions may be also generalized to the case of the plane rectangular lattice with different periods in x- and in y-directions and to the more complicated cases such as, e.g., the (110)-plane in the bcc-structure.

3. Surface roughness

As it is seen from the analysis made above, the magnetic dipolar field from a single atomic layer decreases very fast with the distance from the layer (a typical length of its decay is of the order of the lattice parameter a). It means that the influence of this field may be essential only within a few layers near the surface or the interface. Surface roughness can change the situation. If the typical lateral scale of surface roughness is L, then the typical distance from the rough surface, at which the dipolar field is damped, will be of the order of L. As experimental data show (see, for instance, Ref. [10]), a lateral size of grown islands for MBE-prepared or sputtered films is much more than the lattice parameter. It means that in this case the dipolar field from the rough surface penetrates deep into the magnetic film and, therefore, can influence some of its physical properties. An example of such influence is a recently suggested mechanism for biquadratic interlayer coupling, connected with the dipolar field from magnetic layers with roughness [11].

To evaluate the magnetic dipolar field produced by a rough surface one should add contributions from several imperfect layers. Let us assume that atomic arrangement of the imperfect layer is periodic both in x- and y-directions. In this case the dipolar field from such a layer can be calculated by means of the appropriate additional summations (or integrations at large distances z) in Eqs. (10), (11), in which the parameter a should be set equal to the period of the imperfect structure.

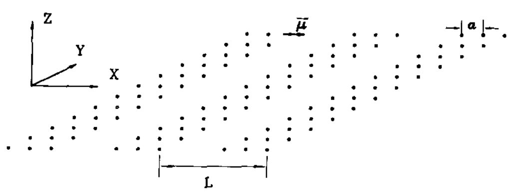

Fig. 2. Imperfect layer corresponding to a rough surface consisting of an array of infinitely long monoatomic terraces and valleys with period L and width $L/2$. The magnetization is supposed to be aligned in x-direction.

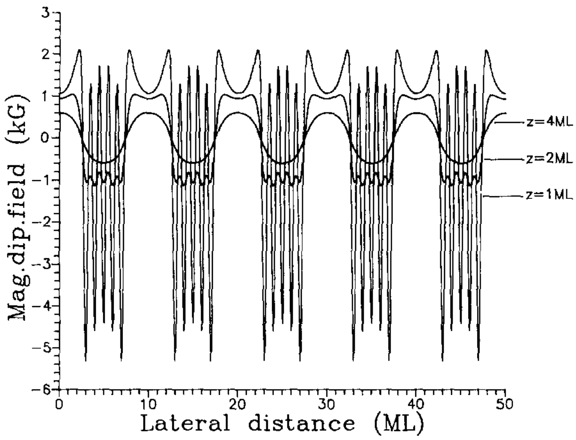

Fig. 3. Calculated profile of the magnetic dipolar field, created by the imperfect layer (Fig. 2) at various distances z for bcc-structure of iron and $L = 10$ ML.

For illustration, let us consider a rough surface consisting of an array of infinitely long monoatomic terraces and valleys with period L and width $L/2$. An imperfect layer corresponding to this roughness is shown in Fig. 2. Let the magnetization be oriented in x-direction. The magnetic dipolar field created by such monoatomic roughness can be evaluated by a summation over x and y of the dipolar fields from the square lattices with the lattice constant L, shifted one relatively to another (see Eq. (10) with $a = L$). The result of this calculation is presented in Fig. 3, where the dipolar field versus x at various distances z from rough surface is shown for bcc-structure of iron and $L = 10$ monolayers (ML). As it is seen, when $z = a/2$ (neighbor plane for bcc structure) short period oscillations connected with the atomic structure of the terraces and localization of spins are distinctly pronounced. These oscillations are modulated by the long period variation of the field caused by periodic roughness. With increasing z the short period oscillations are damped very sharply and only the long period variation of the field remains. In the region of the large distances z one can use an additional integration in Eq. (10) instead of summation. The result of this integration for the structure shown in Fig. 2 can be represented as follows:

$$H_x = -\frac{8\pi\mu}{a^2L}\sum_{k=0}^{\infty}(-1)^{k+1}\cos\left(\frac{2\pi}{L}(2k+1)x\right)\exp\left(-\frac{2\pi}{L}(2k+1)|z|\right), \tag{12a}$$

$$H_y = 0, \tag{12b}$$

$$H_z = \operatorname{sign}(z)\frac{8\pi\mu}{a^2L}\sum_{k=0}^{\infty}(-1)^{k+1}\sin\left(\frac{2\pi}{L}(2k+1)x\right)\exp\left(-\frac{2\pi}{L}(2k+1)|z|\right) \tag{12c}$$

and it practically does not distinguish from the result of the exact summation for $z \geqslant 2a$ and $L \geqslant 4a$. Analogous expressions can be obtained by the corresponding integration in Eq. (11) for the case when the magnetization is aligned perpendicular to the imperfect layer.

Thus, as it is seen from Eq. (12), for large distances from the rough surface the dipolar field decays exponentially with the characteristic length L (the period of the roughness structure), i.e. it penetrates deep into the film material. Using Eqs. (10), (11) more complicated cases of surface roughness can be analyzed.

4. Some applications

Here we present the values of the dipolar fields from the single atomic layer (100) for the bcc-structure, which are essential for calculation of the demagnetizing factors [9], the surface dipolar anisotropy [12] and magnetic hyperfine fields. If the magnetization is aligned within the plane in x-direction, as it follows from Eq. (10), the dipolar field acting on an atom in a lattice site has the only nonvanishing component H_x, i.e. it is oriented along or opposite the direction of the magnetic moments. For the atoms in the neighbor plane $H_x = 0.0831(4\pi M)$, where $M = 2\mu/a^3$ is the magnetization of the film having bcc-structure. For the atoms in the second-neighbor plane $H_x = -0.0065(4\pi M)$, and for the atoms in the third-neighbor plane $H_x = 0.0002(4\pi M)$. The dipolar field acting on an atom in the plane from the rest atoms of this plane is $H_x = 0.1797(4\pi M)$. The total local field at an atom position inside the film is $H_{\parallel} = (4\pi/3)M$. The value of $H_{\parallel}$ is equal to is the sum of the demagnetizing and Lorentz fields of a thin film in a continuous approach.

If the magnetization is aligned perpendicular to the plane in z-direction, as it follows from (11), the only nonzero component of the dipolar field in the points of the atom location is H_z. For atoms in the neighbor plane $H_z = -0.1662(4\pi M)$, for atoms in the second-neighbor plane $H_z = 0.0130(4\pi M)$, and for atoms in the third-neighbor plane $H_z = -0.0005(4\pi M)$. The dipolar field acting on an atom in the plane from the rest atoms of this plane is $H_z = -0.3594(4\pi M)$. The total local field at an atom position inside the film is $H_{\perp} = -(8\pi/3)M$.

4.1. Surface dipolar anisotropy

It is seen that the dipolar field acting on atoms at layers near the surface differ from that in bulk. It results in appearance of the surface dipolar anisotropy, connected with the discreteness of the lattice. The anisotropy energy is given by

$$E_a = (E_{\parallel} - E_{\perp}) \sin^2\theta,$$

where θ is the angle between the normal to the surface and the magnetization. The difference between the magnetostatic energies $E_{\parallel}$ and $E_{\perp}$ can be easily calculated using the values of the dipole fields given above. The result can be written as follows:

$$E_{\parallel} - E_{\perp} = VK_V + SK_S,$$

where V is the volume, $K_V = -(4\pi M^2)/2$ is the usual density of the volume dipolar anisotropy of a thin film, S is the surface area and $K_S = 0.2123(4\pi M^2/2)a/2$ is the density of the surface dipolar anisotropy. For the (100)-surface of iron one obtains $K_S = 0.06$ erg/cm^2, i.e. it is several times less than the values being measured in experiment [1,3]. Note that K_S calculated in [13] for the rough Fe surface (110) has the same order of magnitude. Evaluation of the surface dipole anisotropy caused by the localization of magnetic moments and by surface roughness will be performed elsewhere.

4.2. Hyperfine fields

The opportunity to determine local magnetic hyperfine fields at iron surfaces and interfaces and at layers near to them is offered by CEMS (Conversion Electron Mössbauer Spectroscopy) [2]. The natural linewidth of the Fe^{57} Mössbauer effect is 0.2 mm/s, which corresponds to 12 kG. However, the accuracy of the hyperfine field determination from CEMS data can reach one tenth of the natural linewidth and less, i.e. about 1 kG.

The difference between the dipolar field acting on an atom in bulk and at the surface of iron is approximately 2 kG. It means that the dipolar field gives a visible contribution to the measured values of the hyperfine fields. For the interface Fe/X, where X denotes some substance, the dipolar field may be even several times more than 2 kG, due to, for instance, the large magnetic moment of X (e.g., $\mu = 7\mu_B$ for Gd), or perpendicular orientation of the magnetic moments of iron for very thin films. Moreover, as it is seen from the analysis made above for the bcc-structure and an (100)-interface the dipolar field reveals an oscillating behavior within the Fe film. These oscillations will be damped out at rather small distances (of the order of the lattice parameter). Nevertheless, they can be added to the RKKY-type oscillations of the hyperfine fields observed experimentally for some Fe/X systems [2]. For taking into account these effects consideration of particular cases is necessary.

Another example of the possible influence of the dipolar fields is the effect of the Fe/Gd interface on the observed hyperfine fields which extends up to about 20 ML into the Fe film [14]. In our opinion this long ranging perturbation of the Fe film might be explained by the dipolar fields from a rough Fe/Gd interface due to the large Gd spin moment. Examination of this assumption is subject of future investigations.

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