Micromagnetic theory of domain formation in helimagnets

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We study the necessary conditions for the formation of domains in helimagnets by calculating an exact expression for the classical magnetic dipolar energy associated to the magnetic helix, as a function of its pitch Λ_0 and the system size. For magnets whose caliper dimensions exceed Λ_0, we show that the dipolar energy density vanishes except at a region of depth Λ_0 near the surface of the system. Thus, effectively, the dipolar magnetic energy is a skin effect which scales with the surface of the system. Consequently, the formation of domains becomes, in this case, energetically unfavorable. On the other hand, as the helimagnet smallest caliper dimension becomes comparable to Λ_0, the dipolar energy crossover to a volume effect and, just like in a ferromagnet, for large enough systems the presence of domain walls reduces the dipolar energy and hence induces the formation of domains.

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Helimagnets are magnetic materials exhibiting a space-dependent periodic magnetization in which the atomic spins are ferromagnetic at certain atomic planes but its direction rotates by a small angle as one moves to adjacent layers.[1] The local equilibrium magnetization vector describes a regular helix whose strength and pitch are characteristic of the substance and the temperature. There exist a great variety of materials that display this magnetic behavior such as MnO,[2] different rare-earth elements and compounds,[3] metal silicide alloys,[4,5] magnetic superlattices,[6] two-dimensional electron heterostructure systems with spin-orbit interaction,[7] etc. The helix pitch is usually determined by neutron scattering and typically ranges from a few nanometers for the rare earth to 20–40 nm for the metal silicide compounds. The physical mechanism that accounts for this behavior depends on the system atomic structure and usually arises from competing ferroexchange, antiferroexchange interactions, or from Dzialoshinsky-Moriya antisymmetric spin coupling in structurally asymmetric crystals.[8–11] In the recent years there has been an increasing interest in these systems mainly because of their potential applications in the field of spintronics.[12] The interaction of conduction electrons with the space-dependent exchange field, which couples spin and space degrees of freedom altogether, unveils new mechanisms for the manipulation and control of the electron spin and their currents.

In this work we shall analyze the necessary conditions for domain formation in helimagnets. This is a crucial issue that can have important effects on their applications. In addition, recent experiments employing Lorentz electron microscopy[13] and spin-polarized scanning tunneling microscopy[14] have permitted direct real-space observation of local helical magnetization with a great resolution. Experiments in a monocrystal of $Fe_xCo_{1-x}Si$ report the appearance of complex, nonperiodic, and domainlike structures whose origin remains so far unexplained.[14]

Domain formation in ferromagnets results from the competing effects of the weak but long-ranged magnetostatic dipolar interaction with the strong but short-ranged spin-exchange energy. It is well known that the dipolar energy increases with the volume of the system. The formation of domains reduces the dipolar energy but increases the exchange energy. This latter increase, however, grows with the area of the domain walls and hence is a surface effect. Thus, for large enough systems, the homogeneous magnetization breaks down into the more energetically favorable domain structure.[15] In the following we will analyze the stability of the magnetic helix configuration in the micromagnetic approximation by calculating the resultant magnetic dipolar energy and determining how it increases with the volume. To simplify the mathematics we will assume that the helimagnet has the shape of a long cylinder of radius r_0 and its magnetic helix axis is parallel to the cylinder axis. If we let z be the cylinder axis and call $\Lambda_0=2\pi/\kappa$ as the helix pitch with κ as the associated wave vector, the local magnetization density vector is given by

$$\mathbf{M}(z) = M_0 \begin{pmatrix} \cos \kappa z \\ \sin \kappa z \\ 0 \end{pmatrix} \Theta(r_0 - r), \tag{1}$$

where Θ is the Heaviside step function and r is the radial distance from the z axis. Both M_0 and Λ are constant parameters determined by the minimization of the exchange free-energy functional. Let us calculate the magnetic dipolar energy associated to this configuration. We will first assume the cylinder is very long (infinite) so that end effects are negligible and consider the dipolar energy per unit length. This energy is given by

$$\varepsilon = -\left(\frac{1}{2}\right) \int \int \int \mathbf{M}(\mathbf{r}) \cdot \mathbf{H}(\mathbf{r}) d^3 r, \tag{2}$$

where $\mathbf{H}(\mathbf{r})$ is the field resulting from the magnetization density and the integration extends over a cylinder of unit length. The standard relationships require $\mathbf{H}=\mathbf{B}-4\pi\mathbf{M}$ with $\mathbf{B}$ as the resulting magnetic field and $\mathbf{H}(r)$ satisfying $\nabla \times \mathbf{H}=0$ and $\nabla \cdot \mathbf{H}=-4\pi\nabla\mathbf{M}$. Thus writing $\mathbf{H}(\mathbf{r})=-\nabla\Psi(r)$, we conclude that

$$\nabla^2 \Psi(r) = 4\pi(\nabla \cdot \mathbf{M}) = -4\pi M_0 \cos(\kappa z - \theta)\delta(r - r_0), \tag{3}$$

where we introduced cylindrical coordinates $x=r\cos\theta$ and $y=r\sin\theta$. To solve Eq. (3) we make use of the chiral symmetry corresponding to a magnetic helix. We note that our

system is invariant under arbitrary displacements along the z axis followed by a proper rotation about z. This continuous symmetry leaves the helix and also the cylinder shape uncharged. Consequently, the resulting $\mathbf{H}$ and $\mathbf{B}$ fields must share the same symmetry. Therefore $\mathbf{H}(r)\cdot\mathbf{M}(r)$ is independent of z and the energy integral (2) becomes

$$\varepsilon = -\left(\frac{M_0}{2}\right)\int_0^{r_0} rdr\int_{-\pi}^{+\pi} d\theta H_x(r,\theta). \tag{4}$$

Let us find a solution to Eq. (3) of the form

$$\Psi(r,\theta,z) = f(r)\cos(\kappa z - \theta). \tag{5}$$

Substituting it into Eq. (3), now written in cylindrical coordinates, yields

$$\frac{d^2}{d\rho^2}F(\rho) + \frac{1}{\rho}\frac{d}{d\rho}F - (1+1/\rho^2)F(\rho) = -4\pi(M_0/\kappa)\delta(\rho-\rho_0), \tag{6}$$

where $\rho=\kappa r$ and $f(r)=F(\rho)$. This is the inhomogeneous modified Bessel equation of order 1 and a particular continuous solution and finite for all ρ is

$$F(\rho;\rho_0) = -4\pi(M_0\rho_0/\kappa)\{\Theta(\rho-\rho_0)K_1(\rho)I_1(\rho_0) + \Theta(\rho_0-\rho)K_1(\rho_0)I_1(\rho)\}, \tag{7}$$

where $K_1(\rho)$ and $I_1(\rho)$ are the modified Bessel functions of order 1. On physical grounds, we require that $F(\rho)$ be finite for all r. This condition precludes the addition of any linear combinations of independent solutions of the homogeneous differential equation, namely, $K_1(\rho)$ and $I_1(\rho)$, as they diverge[16] either at $\rho=0$ or $\rho\to\infty$. In conclusion, the solution to Eq. (3) is $\Psi(r,\theta,z)=F(\rho,\rho_0)\cos(\kappa z-\theta)$ with $F(\rho_i\rho_0)$ given by Eq. (7). Let us note that for $r>r_0$ the magnetic field is given by $-\vec{\nabla}\Psi$. So if we substitute for Ψ and take the asymptotic form of the function $K_1(\rho)$ and its derivatives, we conclude that the magnetic field decreases exponentially for large r with a characteristic length κ^{-1}.

It is somewhat surprising that a magnetic field arising from a localized current distribution, as given by $\nabla\times\mathbf{M}$, exhibit for $r\gg 1/\kappa$ an exponentially decaying behavior rather than some inverse power of r, as a multipole expansion approximation would naively indicate. It is precisely the helicity of the current source as well as its infinite length along the z axis which enforces this result. We will show below that this asymptotic behavior of the field has a profound effect on the system magnetostatic energy.

Let us next evaluate the resulting energy. Substituting for $\mathbf{H}=-\nabla\psi$ in Eq. (4) we obtain

$$\varepsilon = (2\pi M_0)^2 K_1(\rho_0)I_1(\rho_0)(\rho_0/\kappa)^2. \tag{8}$$

This will be our main result. First, we consider the limit $r_0 \gg \kappa^{-1}$ for fixed κ. In this case we use the asymptotic expressions for $K_1(\rho)$ and $I_1(\rho)$ for large ρ

$$K_1(\rho) \simeq e^{-\rho}(\pi/2\rho)^{1/2}, \quad I_1(\rho) \simeq e^{\rho}/(2\pi\rho)^{1/2}, \tag{9}$$

so that $K_1(\rho)I_1(\rho)\simeq 1/2\rho_0$, and derive that in this limit the magnetostatic energy grows linearly with r_0. Thus the conclusion is that the dipolar energy does not increase with the volume of the system but rather in proportion to its surface. The origin of this effect will be further discussed below. Let us next consider the limit $\kappa\to 0$ with r_0 fixed. Then have $\rho_0\to 0$ and since $I_1(\rho_0)\simeq\rho_0/2$ and $K_1(\rho_0)\simeq 1/\rho_0$, we obtain $I_1(\rho_0)K_1(\rho_0)\simeq 1/2$. Substituting it into Eq. (8) we conclude that the energy grows as r^2. In summary, we find that in the case κ fixed, $\rho_0\to\infty$, the energy grows as a surface term and hence the system will be stable against domain formation whereas in the latter case, r fixed, $\kappa\to 0$, the system approaches a ferromagnet, the dipolar energy grows as r_0^2, and thus it becomes a volume effect. In Fig. 1 we depict $\varepsilon/(4\pi M_0)^2$ as a function of r_0 and κ. This exhibits the crossover behavior from helimagnet to ferromagnet.

Our next goal is to extend these results to systems with a noncircular cross section. However the lack of chiral symmetry makes this calculation considerably more difficult. Nonetheless we will derive an approximate simple expression for energy. Let us suppose that the system's magnetization is oriented as before but that its cross section is noncircular. We will further assume that its caliper dimensions are much larger than Λ_0 and its length along the z axis is infinite. To obtain the energy per unit length, let us regard the system as composed of many parallel circular cylinders of small radius r_0 that span the whole cross section. The energy is then the sum of the self-energy of each cylinder, as derived before, plus their mutual interactions. A key issue in the evaluation of these terms is to recall that the magnetic field produced by a rod decays exponentially for large r. Thus, for example, we easily derive from Eqs. (5) and (7) that

$$B_x = -\frac{\partial\Psi}{\partial x} = 4\pi M_0\rho_0 I_1(\rho_0)\{K_0(\rho)\cos^2\theta + (1/\rho)K_1(\rho)\cos 2\theta\} \approx M_0\rho_0 I_1(\rho_0)(\pi^3/8\rho)^{1/2}e^{-\rho}\cos^2\theta\ldots, \tag{10}$$

where $K_0(\rho)$ is the modified Bessel function of order 0, for which we substituted by its asymptotic form in the limit $\rho=\kappa r\gg 1$. In Eq. (10) deleted terms are of higher order in $1/\rho$. Similar expressions can be derived for other components of $\mathbf{B}$. The interaction energy of a rod with the rest of the system is given by

$$U_{\text{int}} = -\int\int\int d^3r\,\mathbf{M}\cdot\mathbf{B},$$

$$r>r_0,$$

$$0\le z\le 1. \tag{11}$$

The exponential decay of $\mathbf{B}$ with r allows us to extend the upper limit of the radial integral to ∞ with negligible error. In addition, this limit restores the chiral symmetry of the integral and the integrand becomes independent of z and thus it can be evaluated for any z. Setting $z=0$ and substituting for B_x into Eq. (11), we derive

$$U_{\text{int}} = -\int_0^{2\pi} d\theta \int_{r_0}^{\infty} dr\, rM_0 B_x = 8\pi^2 M_0^2 I_1(\rho_0) K_1(\rho_0)(\rho_0/\kappa)^2. \tag{12}$$

Comparing this result with Eq. (8), we conclude that the interaction energy is twice as large as the rod self-energy and it has the opposite sign. Moreover, we also note that this result is independent of the value of ρ_0. Consequently, the total (bulk) energy of the system given by the sum of the self-energies plus half of their mutual interactions (to avoid double counting) add to zero. This is a surprising effect. The system bulk dipolar magnetic energy vanishes. By comparing it with our previous result, we conclude that part of the energy must have been left out in this analysis. It becomes clear then that the assumptions that lead to Eq. (12) fail when the cylinders lay in the neighborhood of the system boundary surfaces within a characteristic length of order $1/\kappa$. In this case, setting the limit of the integration to infinity is not justified and the correct expression will differ from Eq. (12). Thus we conclude that the total dipolar energy must arise precisely from this boundary region. In fact, by comparing with our previous exact result, we infer that the general expression for the energy must have the form

$$\varepsilon = 2\pi(M_0^2/\kappa)(\text{perimeter of system})c_0, \tag{13}$$

where c_0 is a constant of order 1 that depends on the geometry of the system cross section. Moreover, we note that as the helix pitch grows the region contributing to the surface energy grows accordingly until it comprises the whole system. In this limit the helimagnet becomes a ferromagnet and the dipolar energy increases with the volume.

So far we have analyzed helimagnets of infinite length in the direction of the helix axis. Let us next study the behavior of a system of finite length. However, we will again assume that the pitch Λ_0 is much larger than any caliper dimensions of the magnet. For mathematical simplicity we consider a cylinder of radius r_0 and height L oriented along the helix axis. In addition, let $\kappa L = 2\pi n$, where n is some even integer, $n \gg 1$. The total energy is given by Eq. (2), where the integral extends along the length L; $|z| < L/2$. The field $\mathbf{H}$ must now be calculated for a cylinder of finite length. To calculate $\mathbf{H}$ we evoke the superposition principle and regard the finite cylinder as the sum of an infinite cylinder with magnetization $\mathbf{M}$, as given by Eq. (1), plus a cylinder with a gap of length L, centered at the origin but having the opposite magnetization $-\mathbf{M}$ (see Fig. 2). Thus accordingly, we can write $\mathbf{H} = \mathbf{H}_\infty + \delta\mathbf{H}$ with $\mathbf{H}_\infty$ given by $-\vec{\nabla}\Psi$ and $\delta\mathbf{H}$ being the field at the gap between the separated cylinders. The energy then becomes

$$\varepsilon = -\frac{1}{2}\int_{-L/2}^{+L/2} dz \int_{|r|<r_0} \int \mathbf{M}\cdot\mathbf{H} d^2r = -(2\pi M_0)^2 K_1(\rho_0) I_1(\rho_0) \times (\rho_0/\kappa)^2 L - \frac{1}{2}\int\int\int \mathbf{M}\cdot\delta\mathbf{H}. \tag{14}$$

If we write $\delta\mathbf{H} = -\vec{\nabla}\phi$, the last term in Eq. (14) can be integrated by parts and yields

$$\frac{1}{2}\int\int\int \mathbf{M}\cdot\vec{\nabla}\phi d^3r = \frac{1}{2}\int\int \phi\mathbf{M}\cdot\hat{n}da - \frac{1}{2}\int\int\int \phi\vec{\nabla}\cdot\mathbf{M} d^3r. \tag{15}$$

The first term in Eq. (15) is a surface integral over the cylinder wall at r_0. Inserting the expression for $\vec{\nabla}\mathbf{M}$ into the

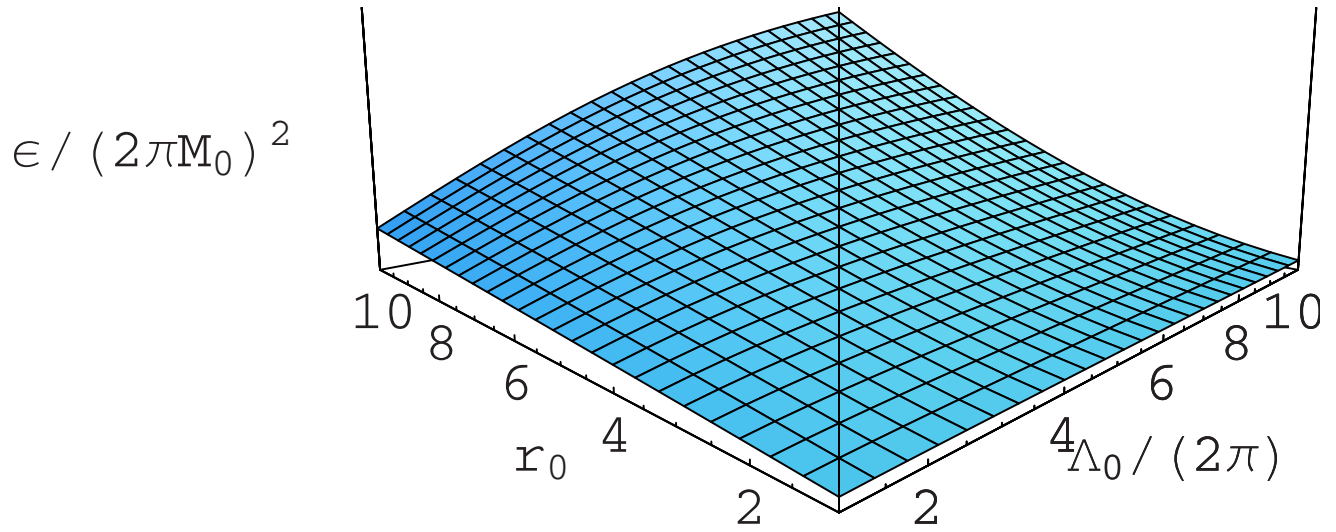

FIG. 1. (Color online) Plot of the magnetic dipolar energy per unit of length of an infinite cylindrical magnet of radius r_0. The magnetization has a constant magnitude M_0, is assumed perpendicular to the cylinder's axis, and rotates about this axis with a period $\Lambda_0 = 2\pi/\kappa$ thus describing a helix. The rescaled energy ε is depicted as function of r_0 and Δ_0. For $\Lambda_0 \ll r_0$ and fixed, the dipolar energy grows linearly with r_0, indicating that it is a surface effect. On the other hand for $\Lambda_0 \gg r_0$ and fixed, the energy grows quadratically with r_0, indicating that it is a volume effect. Note that in this limit the system approaches a ferromagnet. In the intermediate region this graph shows the crossover from one regime to the other. It will be shown in the text that these results are equally valid for a finite length cylinder.

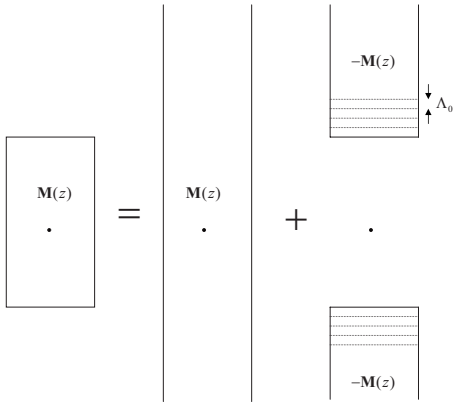

FIG. 2. By the superposition principle, a finite cylinder of length L and magnetization $\mathbf{M}(z)$, as given by Eq. (1) and centered at the origin, can be regarded as the sum of an infinite cylinder with magnetization $\mathbf{M}(z)$ plus an infinite cylinder with magnetization $-\mathbf{M}(z)$, but with a gap of length L centered at the origin. The cylinder sections of length Λ_0 are indicated with dashed lines. Their leading contribution to the magnetic field in the gap is quadrupolar.

second integral gives a contribution identical to the first term. Consequently,

$$-\frac{1}{2}\int\int\int \mathbf{M}\delta\mathbf{H} = 2M_0 r_0 \int_{-L/2}^{L/2} dz \int_{-\pi}^{+\pi} \phi(z,\theta,r_0) \times \cos(\kappa z - \theta) d\theta. \quad (16)$$

To evaluate $\phi(z,\theta,r_0)$ at the gap, $|z| < L/2$, let us slice the top and bottom cylinders into sections of length Λ_0 and calculate their contribution. Clearly ϕ will be given by the sum over all these terms. A slice located at z_0 will consist of a ring of radius r_0, height Λ_0 with a magnetic surface density charge $\sigma(z',\theta) = M_0 \cos(\kappa z' - \theta)$, where $z_0 \le z' \le z_0 + \Lambda_0$, $0 \le \theta \le 2\pi$, and $|z_0| > L/2$. The contribution of each slice will be evaluated approximately by considering its leading nonvanishing multipole expansion term. Let us choose z_0 such that $\kappa z_0 = 2\pi N$, where N is an integer labeling the slice position. It is easily seen that the dipole term vanishes and the quadrupole tensor Q_{ij} has only one nonvanishing component, namely,

$$Q_{yz} = 3\int\int \sigma(z',\theta) y z r_0 d\theta dz' = -3M_0 r_0^2 \pi \Lambda_0/\kappa. \quad (17)$$

Moreover, it is evident that the contribution to $\phi(z,\theta)$ from a slice located at equal distances but in opposite directions will cancel each other. Therefore for $z > 0$ the only contributing slices to $\phi(z,\theta)$ are those located at $L/2 \le z_0 \le L/2 + z$. Similarly for $z < 0$ the contributions result from slices at $-L/2 + z \le z_0 \le -L/2$. Moreover the resulting expression for $\phi(z,\theta)$ must satisfy $\phi(-z,\theta) = -\phi(z,\theta)$. Thus for $z > 0$ the function ϕ is

$$\phi(z,\theta,r_0) = \sum_{\substack{\text{slice at } z_0 \\ \text{with } L/2 \le z_0 \le L/2+z}} 3\pi(\Lambda/\kappa) M_0 r_0^3 \sin\theta (z_0 - z)/[r_0^2 + (z_0 - z)^2]^{5/2} = \pi(M_0 r_0^3/\kappa)\sin\theta \int_{L/2}^{L/2+z} dz_0 [3(z_0 - z)]/[r_0^2 + (z_0 - z)]^{5/2} = \pi(M_0 r_0^3/\kappa)\sin\theta \{[r_0^2 + (L/2 - z)^2]^{-3/2} - [r_0^2 + (L/2)^2]^{-3/2}\}, \quad (18)$$

where we replaced the sum over z_0 by an integral. Finally substituting for $\phi(z,\theta,r_0)$ into Eq. (16), we obtain

$$1/2\int\int\int d^3 r \mathbf{M}\cdot\delta\mathbf{H} = 8\pi^2 (M_0^2 r_0^4/\kappa) \times (1/L^2)\int_0^1 du \sin n\pi u \{[A^2 + (1+u)^2]^{-3/2} + [A^2 + (1-u)^2]^{-3/2}\}, \quad (19)$$

where $A = 2r_0/L$ is the aspect ratio of the cylinder and $\kappa L = 2\pi n$, with n as a large even integer. We can approximate the integral in Eq. (19) by expanding it in inverse powers of n. The rapidly oscillating nature of the integrand implies that as $n \to \infty$, the integral must vanish. Let us then Taylor expand the smooth function inside the curly brackets and integrate the resulting series term by term. If we retain only those which are of order $1/n$, we easily derive

$$1/2\int\int\int d^3 r \mathbf{M}\cdot\delta\mathbf{H} = -(1/8n)(M_0^2 r_0/\kappa)[A^3/(1+A^2)^{3/2}]L + \ldots, \quad (20)$$

where deleted terms are of higher orders in $1/n$. Finally the total energy is obtained by substituting Eq. (20) into Eq. (14). For large r_0, with A and κ fixed, this yields

$$\varepsilon = 2\pi^2 (M_0^2 r_0 L)/\kappa + (1/8n)(M_0^2 r_0 L/\kappa)[A^3/(1+A^2)^{3/2}]. \quad (21)$$

In summary, we have found that the magnetic energy of a finite cylinder is a surface term. Moreover, the contribution resulting from the cylinder end surfaces is negligible. We note, however, this is an exceptional case for which the local magnetization is parallel to the end walls and thus the resulting magnetic charge density vanishes there. We expect that for other geometries or helix axis orientations this will not be the case.

In conclusion, we can generalize our results and state that for any helimagnet whose caliper dimensions are $\gg \Lambda_0$ the magnetic dipolar energy will result from a region of depth Λ_0 located near the surface of the system. Consequently, the magnet will exhibit no domains. Nonetheless, this analysis, in principle, would not preclude the formation of domains confined to the system surface. For example, if the local magnetization gradually becomes tangent to the surface, the magnetic stray field energy would then be reduced. However, in such a case the contribution resulting from the strong exchange anisotropy term will increase in proportion to the

area of the surface-bulk interface, so that domains will not be energetically favorable. These conclusions confirm the conjecture made by Uchida *et al.*[13] that the domain structures observed in the $Fe_xCo_{1-x}Si$ crystal have a nonmagnetic origin. More likely they result from the space dependence of the exchange energy terms associated to inhomogeneity in the distribution of Fe atoms in the samples. Finally we note that systems for which some linear dimension is smaller than Λ_0, such as magnetic nanowires[17,18] or thin magnetic films with free surfaces or embedded in a nonmagnetic host,[14] the exchange energy of a domain wall will scale in proportion to its length; whereas the magnetic dipolar energy grows with the size and hence, for sufficiently large systems, the formation of domains will become energetically favorable. This fact has been amply studied and there exists a vast literature on the subject.[19,20]

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