Ferromagnetic strip domains in an atomic monolayer

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(Received 3 December 1987)

We determine the range of values of the uniaxial surface anisotropy K_s that leads to the formation of domains in an atomic monolayer of ferromagnetically coupled spins. If the ratio f of K_s to the dipolar energy is larger than a minimum value $f_{\min}$ determined by the ratio of exchange to dipolar energies, and if the easy direction is normal to the layer plane, then a domain pattern is energetically favorable compared to any uniformly magnetized configuration. The maximum component of magnetization normal to the layer, $M_\perp$, increases continuously from zero as f increases from its threshold $f_{\min}$ and tends to the saturation magnetization value for large f. Above threshold ($f=f_{\min}$), the width of the domains is very sensitive to the value of f, increasing very rapidly with f and reaching the macroscopic value of the order of 1 cm for a value $f=1.4$. Contrary to the usual assumption of thin domain walls determined by the ratio of exchange to anisotropy energy, in monolayers it is necessary to treat the domain structure as a whole and to include explicitly the dipolar energy. A variational treatment gives, at the threshold of K_s, a simple cosine dependence on distance for the magnetization normal to the layer. The calculation is extended to layers consisting of a few atomic planes.

I. INTRODUCTION

Recently the magnetic properties of ferromagnetic monolayers[1,2] and of films of a few monolayers[3] have become the subject of interest. If there is no anisotropy energy, or if the anisotropy favors alignment in the plane, the dipolar (demagnetizing) field keeps the magnetization in the plane of the layer. Recent calculations,[4] however, show that because of the reduced site symmetry in a monolayer as compared to that of the bulk, the value of the uniaxial surface anisotropy K_s may be substantially enhanced over the bulk value. Recent determinations[5] of K_s (when converted into anisotropy energy per atom) do indeed show values an order of magnitude or more larger than in the bulk. In such a case the magnetization may break into magnetic domains if the easy axis is normal to the layer plane. The purpose of this paper is to investigate (a) the range of values of K_s that, for given magnitudes of the exchange and dipolar energies, will give rise to domain formation and (b) the spatial variation of the magnetization in these domains. We find that a threshold value $K_{s,\min}$ exists, and that when $K_s > K_{s,\min}$ a domain configuration has lower energy than a uniformly magnetized configuration. The effective thickness of the domain wall depends on the width of the domain; it approaches the bulk value only when K_s is well above threshold. Near threshold the width of the domain strips is very sensitive to the value of K_s, increasing very rapidly with increasing K_s. It reaches macroscopic dimensions for a value of the ratio $K_s/K_{s,\min}$ of the order of 1.5 or smaller.

II. DOMAINS OF A MONOLAYER

Since domain formation is driven by a tendency of the spin system to reduce its dipolar energy it is natural to begin by examining the dipolar interaction, first for a uniform spin configuration (magnetized state) and then for a domain configuration. Let $\mathbf{p}$ be the atomic magnetic moment of similar point dipoles, located at the lattice sites $\mathbf{r}=(m\mathbf{e}_x+n\mathbf{e}_y)a_0$, where $\mathbf{e}_z$ and $\mathbf{e}_y$ are unit vectors along the x and y axes and a_0 is the lattice constant. The saturation magnetization is $M_0=p/a_0^3$ and the dipolar energy per unit area for a uniformly magnetized layer is

$$E_d=-\tfrac{1}{2}\mathbf{H}_{\rm loc}\cdot\mathbf{M}_0 a_0 \ .$$

The local field $\mathbf{H}_{\rm loc}$ is obtained from the general expression of the dipolar field at point $\mathbf{r}_i$ exerted by a collection of point dipoles $\mathbf{p}_j$ at points $\mathbf{r}_j$:

$$\mathbf{H}_i=-\left[\frac{\mathbf{p}_j}{r_{ij}^3}-3\frac{\mathbf{r}_{ij}\cdot\mathbf{p}_j\mathbf{r}_{ij}}{r_{ij}^5}\right]\cdots \ , \tag{1}$$

where $r_{ij}=|\,\mathbf{r}_i-\mathbf{r}_j\,|$.

Summing (1) over all sites $j\neq i$ gives the following values for the two cases of interest. (a) $\mathbf{M}_0$ is normal to the layer (configuration $M_{u\perp}$):

$$H_{\rm loc}=H_\perp=-c\left[\frac{8\pi}{3}\right]M_0 \ ,$$

i.e., $H_\perp$ is opposite in direction to M_0. The coefficient $c=1.0782$ is specific to the square lattice and reflects its discreteness. Note that this result is very close to the value $-(8\pi/3)M_0$ which is the local field (the sum of the demagnetizing and Lorentz fields) in a thin film. (b) $\mathbf{M}_0$ is in the plane of the layer (configuration $M_{u\parallel}$):

$$H_\parallel=+c\left[\frac{4\pi}{3}\right]M_0 \ .$$

The difference, $H_\parallel-H_\perp=c4\pi M_0$, is essentially the demagnetizing field in a thin film.

The zero of the energy scale for all magnetic configurations (including domains) will be taken to be the energy of the $M_{u\parallel}$ configuration, so that the energy of the $M_{u\perp}$ configuration becomes

$$E_{d\perp} \rightarrow E_{d\perp} - E_{d\parallel} = c 2\pi M_0^2 a_0 \ . \tag{2}$$

Next, we compare the total energy for the domain and for the $M_{u\parallel}$ and $M_{u\perp}$ configurations. Only domains for which the spin direction is modulated in the x direction but is independent of position along y will be considered (straight domains). The spins on a lattice line that is parallel to the y axis will therefore always be parallel to one another, and such lines can be considered as elementary objects which have a self-energy and an energy of pairwise interaction, both dependent on the direction of the spins, and in terms of which the total dipolar energy of a domain configuration can be calculated. Only Bloch walls, in which the magnetization stays in the yz plane, will be considered. Calculation has shown that the energy of interaction between two lines of dipoles is higher in a Neél-type wall. And finally, the complete calculation will be done only for the case that the maximum value $M_\perp$ of the normal component of magnetization $M_z(x)$ is equal to the saturation value M_0. The case $M_\perp = s\, M_0$ with $s < 1$, which in fact occurs near the threshold of K_s, will be discussed at the end of the section. It can easily be verified that for such homogeneously magnetized lines of spins, each of the three components of the local magnetizations M_x, M_y, and M_z produces only dipolar fields that are, respectively, along the x, y, and z directions.

For the normal component of magnetization M_z the following is true. (a) The field at a lattice site, due to all the other spins on the same line, is

$$H_{zs} = -2M_z \sum_{n=1}^{\infty} \frac{1}{n^3} = -2gM_z \ ,$$

where $g = 1.202\,057$. (b) The field $H_z(n)$ that all the spins on a line parallel to the y axis and having a magnetization M_z exert at a site that is a distance na_0 from that line is found by direct summation. It is given by

$$\begin{aligned} H_z(1) &= -(1.011)2M_z \ , \\ H_2(2) &= -(1.0013)(2M_z/4) \ , \\ H_z(n) &= -(2M_z/n^2) \quad \text{for } n \geq 3 \ . \end{aligned} \tag{3}$$

The last equality is good to better than 0.1% for $n = 3$, and it is exact in the continuum approximation $\sum_n \rightarrow (1/a_0)\int dy$, which is valid for large n. The long-range character exhibited by (3) makes it possible for the weak dipolar interaction to compete with the much stronger but short-range exchange interaction and to give rise to domains having walls in which the magnetization varies slowly on an atomic scale. This slow variation, as will be verified below, makes it possible to incorporate the small deviations of the numerical coefficients of $H_z(1)$ and $H_z(2)$ from unity into the self-field H_{zs} and to use the simple law (3) for all $n \neq 0$. The self-energy becomes

$$E_{zs} = (g + 0.0246)M_z^2 a_0 \ . \tag{4}$$

For the component of magnetization M_y the following is true. (a) The field at a lattice site, due to all the other spins on the same line, is

$$H_{ys} = 4M_y \sum_{n=1}^{\infty} \frac{1}{n^3} = 4gM_y \ . \tag{5}$$

(b) The field $H_\parallel(n)$ at a site due to all the spins on a line parallel to the y axis at a distance na_0 is

$$\begin{aligned} H_\parallel(1) &= -0.1451 M_y \ , \\ H_\parallel(2) &= -0.000\,76 M_y \ , \end{aligned}$$

and for $n \geq 3$, $H_\parallel(n)$ is essentially zero which is the exact result of the continuum approximation. Again, the small values of $H_\parallel(1)$ and $H_\parallel(2)$ can be lumped with the self-energy which, with the help of (4), becomes

$$E_{ys} = -(2g - 0.145\,86)M_y^2 a_0 \ . \tag{6}$$

The coefficient in (6) is precisely $-c(2\pi/3)$, which is the coefficient in the energy $E_{d\parallel}$ of the $M_{u\parallel}$ configuration. To compare the energy of the domain configuration and those of the uniform spin configurations, the same zero of energy must be used in both, i.e., $E_{d\parallel}$ must be subtracted from the energy. From $M_y^2 = M_0^2 - M_z^2$ the quantity M_y^2 can be eliminated and the self-energy of the domain configuration per unit area becomes

$$\begin{aligned} E_{ds} &= E_{zs} + E_{ys} - E_{d\parallel} \\ &= qM_z^2 a_0 \ , \end{aligned} \tag{7}$$

where $q = (3g - 0.121\,26)$. The reason small contributions to q are kept here is that it will be found below that energy differences between domain and uniform spin configurations are very small, so that neglect of small quantities here could lead to serious error.

The interaction energy between two lines of spins at $x = na_0$ and $x' = n'a_0$ is

$$E_{di}(n,n') = \frac{M_z(n)M_z(n')}{(n-n')^2} \ . \tag{8}$$

It may be possible to do an exact calculation based on (7) and (8), but instead we will assume a simple domain shape depending on two parameters a and δ which are essentially the width of the domain and the ratio of the wall thickness to the domain width, and we will determine the values of a and δ by minimizing the total energy. The assumed profile of the normal component of magnetization is shown in Fig. 1: $M_z(x)$ is constant and equal to $M_\perp$ ($M_\perp = M_0$ here) in regions of width d, and it varies according to $\cos(\pi x/w)$ in regions of width w where the magnetization turns in the yz plane at the rate π/w. The half periodicity of the structure is $a = d + w$ and δ is defined as $\delta = w/a$. For brevity, a will be referred to as the domain width, and $w = a\delta$ will be called the domain-wall thickness, although the customary definition[6] of the thickness is in terms of the slope dM_z/dx at the point where $M_z = 0$, and thus corresponds to $(2/\pi)w$. The dipolar energy per unit area can now be calculated.

The line self-energy (7) is given by the average value of

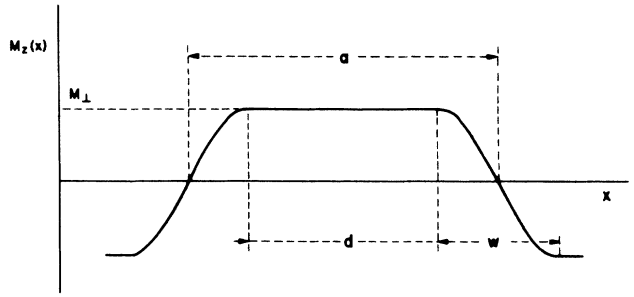

FIG. 1. Assumed shape of the domains in an atomic monolayer. $M_z(x)$ varies as $\cos(\pi x/w)$ in the wall regions. The values of a and of $\delta=(w/a)$ are determined variationally.

$M_z(x)^2$ over the profile of Fig. 1 and this is simply $M_0^2(1-\delta)+\frac{1}{2}M_0^2\delta$: The first term is M_0^2 weighted by the fraction $(1-\delta)$ of the layer area over which $M_z(x)$ is constant, and the second is the average of $[M_0\cos(\pi x/w)]^2$ weighted by the fraction δ of the area over which the magnetization varies. Thus

$$\langle E_{ds}\rangle = q(1-\delta/2)M_0^2 a_0 \ . \tag{9}$$

To calculate the average of E_{di} the magnetization of Fig. 1 is expanded into a cosine Fourier series with only odd harmonics:

$$M_z(x)=M_0 \sum_{m=1,3,\ldots} b_m \cos(m\pi x/a) \ , \tag{10}$$

where

$$b_m=(-1)^{(m-1)/2}\frac{4}{\pi m}\frac{1}{1-m^2\delta^2}\cos\left[\frac{\pi}{2}m\delta\right] \ . \tag{11}$$

The desired average is

$$\langle E_{di}\rangle=\frac{1}{2l}\sum_n \sum_{n'\neq n}\frac{M_z(n)M_z(n')}{(n-n')^2}a_0 \ , \tag{12}$$

where $2la_0$ is the dimension of the monolayer in the x direction, the sums over n and n' range from $-l$ to l and the limit $l\to\infty$ is taken. Anticipating that a and w will turn out to be large compared to a_0, the continuum approximation is made and the sums over n and n' are replaced by integrals over $x=na_0$ and $x'=n'a_0$. The product

$$\cos(m\pi x/a)\cos(m'\pi x'/a)$$

is expressed as a sum of cosines of the sum and difference of the arguments and new coordinates $X=(x+x')/2$ and $u=(x-x')$ are defined. The lower limit on u that corresponds to $n'=n\pm1$ is $u_{\min}=\alpha a_0$, where $\alpha=6/\pi^2$, as follows from the fact that $\sum_n(1/n^2)=\pi^2/6$. The integration over X gives zero unless $m=m'$ and one obtains

$$\langle E_{di}\rangle=M_0^2a_0^2\sum_{m=1,3,\ldots} b_m^2\int_{\alpha a_0}^{\infty}\frac{\cos(m\pi u/a)}{u^2}du \ . \tag{13}$$

This is actually valid for any domain shape if the appropriate coefficients b_m are used. Integrating by parts and keeping only sums first order in (a_0/a), one finally obtains

$$\langle E_{di}\rangle=M_0^2a_0\left[\frac{\pi^2}{6}\sum_m b_m^2-\frac{\pi}{2}ka_0\sum_m mb_m^2\right] \ , \tag{14}$$

where $k=\pi/a$. The first sum in (14) can be written down immediately since, from (10), it is proportional to the average value $\langle M_z(x)^2\rangle$. Thus

$$\sum_{m=1,3,\ldots} b_m^2=\frac{2\langle M_z(x)\rangle^2}{M_0^2}=2-\delta \ . \tag{15}$$

The second sum cannot be evaluated in closed form. It will be denoted by

$$G(\delta)=\sum_{m=1,3,\ldots} mb_m(\delta)^2 \ . \tag{16}$$

The sum of (9) and (14) gives the total dipolar energy. Note that the sum $q+\pi^2/3$ is exactly equal to $2\pi c$, which is the coefficient in the dipolar energy of the $M_{u\perp}$ configuration, Eq. (2). The result is

$$\langle E_d\rangle=c2\pi M_0^2a_0(1-\delta/2)-(\pi/2)M_0^2a_0(ka_0)G(\delta) \ . \tag{17}$$

This reduces correctly to the energy (2) in the limit $\delta\to0$, $k\to0$.

We consider next the anisotropy and exchange energies. The former is written as $E_a=-\frac{1}{2}K_s\cos^2\theta$, where θ is the angle between the magnetization and the normal to the layer plane. Note that K_s differs in magnitude (by a factor of $\frac{1}{2}$) and in sign from the same quantity defined in Ref. 5. Only positive K_s may lead to domains. The averaged uniaxial anisotropy for the domains of Fig. 1 is

$$\langle E_a\rangle=-\tfrac{1}{2}K_s[1-(\delta/2)] \ . \tag{18}$$

The local exchange energy per unit area, relative to the $M_{u\parallel}$ spin configuration is

$$E_{\rm ex}=\frac{1}{2}\frac{A}{a_0}\left[\frac{d\theta}{dxa_0}\right]^2 \ ,$$

where $A=(2JS^2/a_0)$ and $2JS^2$ is the interaction energy between nearest neighbors. Substituting $(d\theta/dx)=(\pi/w)=(k/\delta)$ over the fractional area δ occupied by the domain wall, and $(d\theta/dx)=0$ over the part where the magnetization is constant, the average of $E_{\rm ex}$ becomes

$$\langle E_{\rm ex}\rangle=\frac{1}{2\delta}\frac{A}{a_0}(ka_0)^2 \ . \tag{19}$$

The total energy E_t is the sum of (17), (18), and (19) and is to be minimized with respect to $k=(\pi/a)$ and to δ. Let $E_0=2\pi M_0^2a_0$. We define the dimensionless quantities

$$R=\frac{A/a_0}{E_0}, \quad f=\frac{K_s}{2cE_0}, \quad e_t=\frac{E_t}{E_0} \ .$$

Typically R is quite large ($R=25$ is close to the value for gadolinium; for iron, R is of the order of 140) while f may range from zero to the order of unity. The expression for e_t is

$$e_t(\delta,a)=c(1-f)\left[1-\frac{\delta}{2}\right]-\tfrac{1}{4}(ka_0)G(\delta)+\frac{R}{2\delta}(ka_0)^2 , \tag{20}$$

where $G(\delta)$ is given in (16).

The minimization conditions are

$$\frac{\partial e_t}{\partial(ka_0)}=-\tfrac{1}{4}G(\delta)+\frac{R}{\delta}(ka_0)=0 , \tag{21}$$

$$\frac{\partial e_t}{\partial\delta}=-\frac{c}{2}(1-f)-\tfrac{1}{4}(ka_0)\frac{dG}{d\delta}-\frac{R}{2\delta^2}(ka_0)^2=0 . \tag{22}$$

Equation (21) gives the domain width $a=(\pi/k)$ in terms of δ,

$$\frac{a}{a_0}=\frac{4\pi R}{\delta G(\delta)} , \tag{23}$$

and substitution of (23) into (22) gives the relation between δ and the physical parameters f and R:

$$f=1+\frac{G(\delta)[G(\delta)+2\delta(dG/d\delta)]}{16cR} . \tag{24}$$

This equation cannot be solved for δ in terms of f but examination of $G(\delta)$ reveals the properties of this function which are sufficient to characterize the domains. (a) From (16) and (11) it can easily be seen that $G(1)=1$ and $(dG/d\delta)_{\delta=1}=-1$. (b) Numerical evaluation of (16) shows that as δ decreases from 1 in the range (1–0), the function $G(\delta)$ increases monotonically while $(dG/d\delta)$ remains negative and its absolute value increases monotonically and faster than that of $G(\delta)$. The product $\delta G(\delta)$ decreases uniformly in the same range. (c) The limiting behavior of $G(\delta)$ as δ approaches zero is found by replacing the summation of the series by an integration (continuum approximation with $m\delta\rightarrow x$). The result is

$$\lim_{\delta\rightarrow 0}G(\delta)=\frac{8}{\pi^2}\ln\frac{1}{\delta}+0.075\,67, \quad \frac{dG}{d\delta}=-\frac{8}{\pi^2}\frac{1}{\delta} . \tag{25}$$

Equation (25) is accurate to 2×10^{-3} for $\delta\leq 0.1$.

These properties of $G(\delta)$ and $dG/d\delta$ determine the shapes and the energies of domains in monolayers.

(a) From (24) and the properties of $G(\delta)$ discussed above, it follows that the minimum value $f=f_{\min}$ for which domains will occur corresponds to $\delta=1$:

$$f_{\min}=1-(1/16cR) . \tag{26}$$

As δ decreases from 1, the right-hand side (rhs) of (24) increases uniformly. Note that the deviation of $f_{\min}$ from unity is very small since the ratio R of exchange to dipolar energy is large. The value $R=25$ will henceforth be assumed for numerical purposes, so that $f_{\min}=0.9977$. From (23), the corresponding value of the domain width in terms of the lattice constant is $(a/a_0)=4\pi R=10^2\pi$. The total energy of the $M_{u\perp}$ configuration at $f=f_{\min}$ is $e_t(u\perp)=c(1-f)=(1/16R)$ while the total energy (20) of the domain configuration is zero, and thus degenerate with the energy of the $M_{u\parallel}$ configuration. As f increases from $f_{\min}$ the domain configuration becomes the energetically stable one. Note that at $\delta=1$ *the shape of the domain is purely cosine-like,* i.e., the flat part of Fig. 1 has shrunk to zero and, loosely speaking, the whole domain structure consists of domain walls. This curious behavior occurs because the strong exchange energy, which depends quadratically on the wave vector k, competes only with the weak dipolar energy. The exchange energy of each Fourier component of the magnetization, $b_n\cos(nkx)$, is proportional to n^2, and hence the minimum occurs if only the component $n=1$ is present.

From (23) it follows that as δ decreases the value of a increases and the value of f as given by (24) increases. Physically, this relation between f and a expresses the fact that an increase in the uniaxial anisotropy tends to increase the mean square value $\langle M_z(x)^2\rangle$ in order to minimize the total energy, and thus leads to a wider flat region in Fig. 1. At the same time the increased anisotropy makes the wall region narrower and thus decreases the width $w=a\delta$. The quantities a and w, expressed in units of the lattice constant, have been calculated numerically. They are shown in Fig. 2 for a range of values of $f>f_{\min}$ and for the corresponding values of δ. It is seen that a change in δ by two orders of magnitude corresponds to a change in f of only 4%. This extreme sensitivity of the domain pattern to changes in f occurs because in two-dimensional (2D) systems (as opposed to 3D), domain formation can achieve only a very small reduction in the total energy on the scale of E_0. When the anisotropy ratio f is even a little larger than 1, the flat region of Fig. 1 is so large on an atomic scale that in spite of its long-range character, the deviation from E_0 of the dipolar energy is only minimal. Hence minor changes in f produce very large changes in domain width and therefore in δ. Table I gives the values of $G(\delta)$, $dG/d\delta$, and f as δ ranges over four decades.

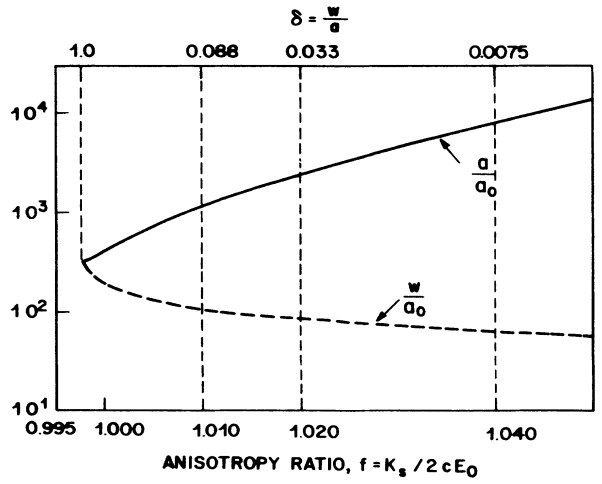

FIG. 2. Values of the domain width a and of the wall thickness w, expressed in units of the lattice constant, as functions of the uniaxial anisotropy in atomic monolayers.

TABLE I. Range of $G(\delta)$, $dG/d\delta$, and f as δ varies from 1 to 10^{-4}. The value of R used in the expression of f is $R=25$.

δ	$G(\delta)$	$\frac{dG}{d\delta}$	f
1.0	1.0	−1.0	0.997 6
10^{-1}	2.941 45	−8.118 23	1.009 0
10^{-2}	4.808 48	−81.057 4	1.035 5
10^{-3}	6.674 89	−810.574	1.078 2
10^{-4}	8.541 30	−8105.74	1.137 05

It is of interest to find the value of f for which the domain size is of macroscopic dimensions, e.g., $(a/a_0)=10^8$. Equation (23) gives $\delta\sim 2\times 10^{-7}$ and correspondingly $f_{\max}\sim 1.4$. In practice, domains will therefore be observable only in the range $f_{\min}\le f\le f_{\max}$ while in principle, as will be seen below, *the domain configuration is lowest in energy for arbitrarily large f.*

(b) The binding energy $e_\perp$ of the domain structure is defined as the difference between the energy of the lowest uniform spin configuration and that of the domain structure. Hence

$$e_b=-e_t(\delta,a) \quad \text{for } f<1 ,$$

$$e_b=c(1-f)-e_t(\delta,a) \quad \text{for } f>1 .$$

For $f_{\min}<f\le 1$, e_b is positive and reaches its maximum value at $f=1$, corresponding to $\delta=0.4663$ and $G(\delta)=1.6799$ independently of the value of R. The binding energy is $e_{b,\max}=(1/32R)\delta G(\delta)^2=16.45\times 10^{-4}$ for $R=25$. For $f>1$, the expression for e_b is obtained from (20), (23), and (24):

$$e_b=-\frac{\delta^2 G(\delta)\,dG/d\delta}{16R} . \tag{27}$$

Since $dG/d\delta$ is negative for all δ, e_b is positive for all $f>1$. This proves that the domain configuration has *lower energy* than the uniformly magnetized configuration *for all values* $K_s>K_{x,\min}$. Figure 3 shows a plot of e_b versus f in units of $(10^{-4})2\pi M_0^2 a_0$. Because e_b is so small, the saturation field, even at $e_{b,\max}$ is very small, of the order $(e_{b,\max}/M_0 a_0)\approx 10^{-2}M_0$, about 20 Oe.

The limiting expression for the wall width w_l as $f\to\infty$ is obtained from (24) and (23):

$$w_l=\frac{4\pi R a_0}{(16cRf)^{1/2}}=\pi\left[\frac{2A/a_0}{K_s}\right]^{1/2} . \tag{28}$$

Multiplying by $(2/\pi)$ to conform to the usual definition of the width, $(2/\pi)w_l$ is a factor $(2\sqrt{2}/\pi)\sim 0.9$ smaller than the exact value of the width at the center of the wall.[6] For the value $f=f_{\max}$ that corresponds to the macroscopic dimension $a=10^8 a_0$, w equals $20a_0$ while the value of (28) for the same f is $w_l=12.7a_0$. Thus, in practice, the limiting expression for w is not attained in monolayers, which is not surprising since $f_{\max}\sim 1.4$ is not a large number.

In the preceding calculation the value of $M_\perp$ in Fig. 1 has been taken equal to the saturation value M_0. More

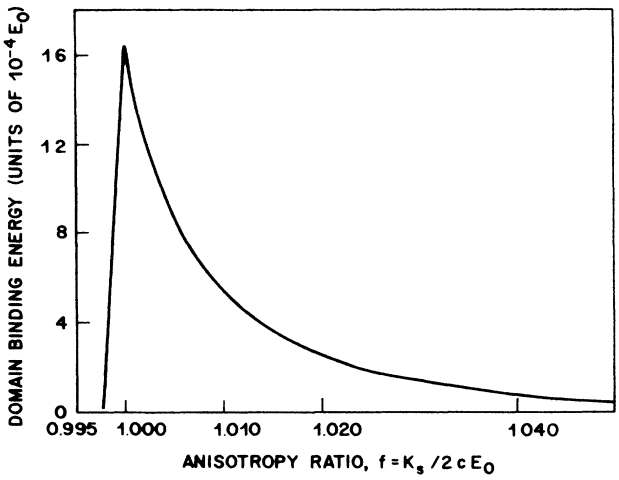

FIG. 3. Domain binding energy per unit area as a function of the uniaxial anisotropy.

generally $M_\perp$ may be smaller, $M_\perp=sM_0$, where $s<1$. The dipolar, anisotropy, and exchange energies are modified as follows. (a) Both (7) and (8) are proportional to M_z^2, hence E_d acquires a factor s^2. (b) The anisotropy energy E_a also acquires a factor s^2 since it is proportional to $\cos^2\theta$. (c) E_{ex} is a little more complicated: In the region of the wall, θ depends on distance as

$$\cos\theta=s\cos(\pi x/w) ,$$

so that

$$\left[\frac{d\theta}{dx}\right]^2=\frac{s^2(\pi/w)^2\sin^2(\pi x/w)}{1-s^2\cos^2(\pi x/w)} . \tag{29}$$

The exchange energy is obtained by averaging (29) over the width w and multiplying by δ. The result is

$$\langle E_{ex}\rangle=\frac{1}{2\delta}\frac{A}{a_0}(ka_0)^2[1-(1-s^2)^{1/2}] . \tag{30}$$

Since below the anisotropy threshold the magnetization lies in the layer plane, it is to be expected that at threshold the value of s will start from zero so as to allow a gradual development of the normal component of the magnetization. For $s\to 0$, the bracket in (30) reduces to $s^2/2$. Since E_d and E_a are reduced by s^2, the overall effect of a small s is to make the exchange appear a factor of 2 smaller, so that R is replaced by $R/2$. The value of $f_{\min}$ as $s\to 0$ is, correspondingly,

$$f_{\min}=1-(1/8cR) . \tag{31}$$

Since this value is smaller than (26) it is the true threshold for domain formation. As f increases from this value, s is expected to increase and to approach unity for "large" f. A variational calculation similar to the preceding one but depending also on s could be made to obtain more complete results.

III. DOMAINS IN THIN FILMS

There has been a considerable amount of work done on this subject; since it is likely that the current interest in thin films of only a few atomic planes will lead to studies of their dynamic as well as static properties, a short list of representative references[7-13] may be useful. The purpose of this section is twofold: (1) To verify that the treatment of domain formation in a monolayer can be obtained as the limit of a corresponding treatment in thin films, and (2) to generalize in a simple way the previous calculation to the case of films a few monolayers thick, but of thickness still small compared to the characteristic length.[8] A variational treatment of the domain structure, different from ours, has previously been given by Kaczer *et al.*[8] We found it difficult to compare our results with theirs, partly because they consider mostly thicker films and specific values of the anisotropy while we emphasize the dependence of the domain structure on the magnitude of the anisotropy and on the number (small) of atomic layers.

To make a comparison with Sec. II possible, we assume that the anisotropy energy per *atom*, Ka_0^3, is the same in the film as it is in the monolayer so that $K_s = Ka_0$. This is certainly not true in physical systems, and it is expected that in fact $K_s \gg Ka_0$. As a result, in actual systems the magnetization will not be uniform in the z direction and our simple model of a z-independent M_z will fail in the limit of small t. It is with these provisions that our treatment of the small t limit must be understood.

The dipolar energy E_d per unit area of the film is calculated from the magnetostatic potential $\psi(x,z)$ of the moment distribution. $\psi(x,z)$ is periodic with period $2a$ in the x direction and it is odd with respect to z since its sources are $\pm 4\pi M_z(x)$ at $z = \pm t$. As in Sec. II the calculation is done only for $M_\perp = M_0$ with the understanding that the value of $M_\perp$ will develop gradually from zero as the anisotropy increases, and that at threshold this can be taken into account by letting $A \to A/2$. Following standard methods[14] the dipolar energy can be shown to be given by

$$E_d = M_0^2 a \sum_{m=1,3,\ldots} \frac{1}{m} b_m^2(\delta) \left[1 - \exp\left[-2\pi m \frac{t}{a} \right] \right] , \tag{32}$$

where $b_m(\delta)$ is given in (11). In analogy to (18) and (19) the anisotropy and exchange energies per unit area are given by

$$E_a = -\tfrac{1}{2} K [1 - (\delta/2)] 2t , \tag{33}$$

$$E_{ex} = \frac{\pi^2}{2\delta} \frac{A}{a^2} 2t . \tag{34}$$

The total energy E_t is the sum of E_d, E_a, and E_{ez} and it depends, for given t, on the same parameters a and δ as in Sec. II. The monolayer limit corresponds to the value $2t = a_0$. To determine a and δ we define a dimensionless energy $e_t = (E_t/E_0)$, where $E_0 = 2\pi M_0^2 a_0$, and solve the two variational equations $(\partial e_t/\partial a) = 0$ and $(\partial e_t/\partial \delta) = 0$.

For $(t/a) \ll 1$ the exponential in (32) is expanded to second order in t/a. The first-order term brings down a factor m which converts the sum over m into $\sum b_m^2$, or $(2-\delta)$. The second-order term likewise brings a factor m^2, which converts the corresponding sum into $G(\delta)$. Defining $f = (K/4\pi M_0^2)$ and $R = (A/a_0 E_0)$ as before, we obtain

$$e_t = \left[1 - \frac{\delta}{2} \right] \frac{2t}{a_0} - \tfrac{1}{4} G(\delta) k a_0 \left[\frac{2t}{a_0} \right]^2 - \left[1 - \frac{\delta}{2} \right] f \left[\frac{2t}{a_0} \right] + \frac{R}{2\delta} (k a_0)^2 \left[\frac{2t}{a_0} \right] . \tag{35}$$

Note the similarity of (35) to (20): In the monolayer limit $2t = a_0$, Eq. (35) reduces exactly to the monolayer result (20), except that the factor $c = 1.0782$ which reflected the discreteness of the square lattice is absent. This was to be expected since we are assuming here a continuous film. Equation (35) shows that if one is willing to neglect the small difference between the factor c and unity, the monolayer case can be obtained as the limit of a thin-film calculation.

Next we examine the dependence of the domain size a and of the anisotropy threshold $f_{\min}$ on n, the number of atomic layers in the film. Substituting $(2t/a_0) = n$ and $k = (\pi/a)$ in (35) we find

$$e_t = (1-f) \left[1 - \frac{\delta}{2} \right] n - \tfrac{1}{4} G(\delta) \left[\frac{\pi a_0}{a} \right] n^2 + \frac{R}{2\delta} \left[\frac{\pi a_0}{a} \right]^2 n . \tag{36}$$

The variational equation $(\partial e_t/\partial a) = 0$ gives

$$\frac{a}{a_0} = \frac{1}{n} \frac{4\pi R}{\delta G(\delta)} . \tag{37}$$

Thus at fixed δ the half-periodicity a is inversely proportional to the number of atomic layers. This is a consequence of the fact that the long-range part (and only that part) of the dipolar field at a lattice site in an n-layer film is proportional to n.

The value of $f_{\min}$ is found by substituting (37) in the second variational equation, $(\partial e_t/\partial \delta) = 0$. The result for f is

$$f = 1 + \frac{n^2}{16R} G(\delta) \left[G(\delta) + 2\delta \left[\frac{dG}{d\delta} \right] \right] , \tag{38}$$

which is the same as Eq. (24) except for the factor n^2. By the same argument as in Sec. II, the minimum value $f_{\min}$ occurs for $\delta = 1$, and at threshold the magnetization $M_z(x)$ varies as $\cos(\pi x/z)$. $f_{\min}$ is given by

$$f_{\min} = 1 - (n^2/16R) . \tag{39}$$

The factor n^2 in (39) can be understood as the combined effects of (a) the long-range dipolar field at a site being proportional to n for a fixed domain width a and (b) the width a being inversely proportional to n as it follows from (37). Equation (39) states that at threshold the an-

isotropy constant is the sum of the demagnetizing energy $2\pi M_0^2$ and the exchange energy [last term of (36)], plus the third term of (36) which is the reduction in dipolar energy due to domain formation.

IV. SUMMARY

A variational treatment of domain formation in monolayers and in films of a few monolayers has been given. It shows that when the surface anisotropy K_s is larger than a threshold value which, for films up to two monolayers thick, depends only on the ratio of exchange to dipolar energy, a domain structure with magnetization normal to the layer plane is energetically favored. (The easy direction given by K_s must of course be normal to the layer plane.) Near the threshold of K_s the width of the domains is very sensitive to the value of K_s and increases rapidly with K_s. If in the more-than-two-layer case one assumes an anisotropy energy per atom that is the same throughout the film, then the result for an n-layer film scales simply with n to the monolayer case [Eqs. (37) and (38)]. Much remains to be done in this field, such as the treatment of a physical model more realistic than that of point dipoles, an allowance for a variable anisotropy energy that depends on position of the atomic layer in the film, and a treatment of the gradual increase of $M_\perp$ above threshold.

Note added. After this calculation was completed it was suggested by J. Villain (private communication) that checker-board domains may lead to still lower energies. Dr. J. Villain pointed out to one of us (Y.Y.) that for very large f one should obtain the Ising limit. Doing a calculation on a *discrete* lattice he estimated that in the Ising limit (infinite K_s) the width of the domain strips in units of the lattice constant would be of the order $\exp(4\pi R)$. In the large K_s limit our continuum model breaks down when the wall thickness becomes of the order of the lattice constant a_0. From Eqs. (23) and (24) this happens when $f=\pi^2 R$. The corresponding domain width is $(a/a_0)=\exp(\pi^3 R/2)$, in agreement with Villain's result to within a coefficient. Our continuum model thus breaks down when $f \gtrsim \pi^2 R$, which is of the order of 10^2.

ACKNOWLEDGMENTS

It is a pleasure to thank R. Wolfe for stimulating discussions, Professor B. Heinrich for sending a copy of his work before publication, and Professor J. Villain for his interest and for communicating his results before publication.

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