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A Generalization of the Demagnetizing Tensor for Nonuniform Magnetization

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The demagnetizing tensor for ferromagnets is generalized to include interactions between uniformly magnetized bodies. This "mutual" demagnetizing tensor is symmetric, has a trace of zero, and has other simple geometric properties. The tensor is then used to develop an expression for the macroscopic magnetic field in non-uniformly magnetized bodies of arbitrary shape. Finally, the theory is applied to a block model of magnetization and explicit formulae for the tensor components are given.

INTRODUCTION

New techniques such as the interference-contrast colloid technique [*Hartmann*, 1987*a*] and magnetic force microscopy [*Hartmann*, 1990*a*; *Williams et al.*, 1992] are making it possible to investigate the domain structure of ferromagnetic or ferrimagnetic bodies in much greater detail than previously. For a full interpretation of these observations, however, it is necessary to know how the surface field depends on the domain structure. So far, calculations of the surface field have relied on fairly crude models of the domain walls (as pointed out in *Hartmann* [1990*b*]), despite the fact that sophisticated two- and three-dimensional micromagnetic models of the magnetization in ferromagnets have been developed by several researchers [e.g., *Fredkin and Koehler*, 1987; *Schabes and Aharoni*, 1987; *Williams and Dunlop*, 1989].

The internal magnetic field and demagnetizing energy of a uniformly magnetized body can be conveniently expressed in terms of a demagnetizing tensor. In an ellipsoidal body,

$$\boldsymbol{H} = -\boldsymbol{N}\cdot\boldsymbol{M} \tag{1}$$

holds exactly [e.g., *Brown*, 1962], where $\boldsymbol{H}$ is the field due to the magnetization, $\boldsymbol{M}$ is the magnetization, and $\boldsymbol{N}$ is the demagnetizing tensor. $\boldsymbol{N}$ depends only on the lengths and orientations of the principal axes of the ellipsoid. The demagnetizing energy is

$$E_d = -\frac{\mu_0}{2}\boldsymbol{M}\cdot\boldsymbol{H}\,\tau, \tag{2}$$

where τ is the volume of the body.

In general, a uniformly magnetized body does not have a uniform internal field. It can be shown that if $\boldsymbol{H}$ is replaced by a uniform average field $<\boldsymbol{H}>_\tau$, there is still a demagnetizing tensor such that equation (1) holds, and in some respects the behavior of such a body is equivalent to that of an ellipsoidal body with appropriate dimensions [*Brown*, 1962]. Three-dimensional micromagnetic calculations have shown, however, that the magnetization is not really uniform even in particles where there is only one domain [*Williams and Dunlop*, 1989].

In this paper it is shown how the demagnetizing tensor can be generalized to give a simple expression for the field (internal or external) due to a given magnetization pattern.

GENERAL TENSOR FORMULATION

Two Uniformly Magnetized Bodies

In a ferromagnetic body, $\nabla\times\boldsymbol{H}=0$ and $\nabla\cdot\boldsymbol{B}=0$. The magnetic field is therefore the gradient of a potential:

$$\boldsymbol{H} = -\nabla\Phi_M, \tag{3}$$

where the scalar potential Φ_M is determined by the magnetization:

$$\Phi_M(\boldsymbol{r}) = \frac{1}{4\pi}\int \boldsymbol{M}(\boldsymbol{r}')\cdot\nabla'\Big(\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\Big)d\tau' \tag{4}$$

[e.g., *Jackson*, 1975]; here ∇' is the gradient with respect to $\boldsymbol{r}'$. If the body is uniformly magnetized, then

$$\Phi_M(\boldsymbol{r}) = \frac{1}{4\pi}\boldsymbol{M}'\cdot\int_{\tau'}\nabla'\Big(\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\Big)d\tau', \tag{5}$$

where the integration is over the magnetized region. If τ is another volume (which may overlap τ' or even coincide with it), then the average field in τ is

$$<\boldsymbol{H}'>_\tau = \frac{1}{\tau}\int_\tau(-\nabla\Phi_M)d\tau = -\boldsymbol{M}'\cdot\boldsymbol{N}, \tag{6}$$

where

$$N_{ij} = -\frac{1}{4\pi\tau}\int_\tau d\tau\int_{\tau'}\nabla_i'\nabla_j'\Big(\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\Big)d\tau' \tag{7}$$

(using the fact that $\nabla(1/|\boldsymbol{r}-\boldsymbol{r}'|) = -\nabla'(1/|\boldsymbol{r}-\boldsymbol{r}'|)$). The energy in the volume τ due to the field $\boldsymbol{H}'$ is

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$$E_d = -\frac{\mu_0}{2} \boldsymbol{M} \cdot \boldsymbol{N} \cdot \boldsymbol{M}' \tau. \tag{8}$$

The tensor $\boldsymbol{N}$ has some simple properties. Clearly it is symmetric; also, because it is dimensionless, it is unchanged if all quantities are scaled by the same amount. The trace is

$$tr(\boldsymbol{N}) = -\frac{1}{4\pi\tau} \int_\tau d\tau \int_{\tau'} \nabla'^2 \left(\frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|}\right) d\tau'. \tag{9}$$

Since $\nabla'^2(1/|\boldsymbol{r} - \boldsymbol{r}'|) = -4\pi\delta(\boldsymbol{r} - \boldsymbol{r}')$ [*Jackson*, 1975, p. 40], this integral is the fraction of the volume τ which overlaps τ'. If the two volumes τ and τ' coincide, $\boldsymbol{N}$ is the ordinary demagnetizing tensor and $tr(\boldsymbol{N}) = 1$; if they do not overlap, $\boldsymbol{N}$ has zero trace. Since these two cases are analogous to self-induction and mutual induction of current loops, we will call $\boldsymbol{N}$ the self-demagnetizing tensor if τ and τ' coincide and the mutual demagnetizing tensor if they are discrete.

By choosing reference coordinates $\boldsymbol{r}_0$ in τ and $\boldsymbol{r}'_0$ in τ' (e.g., center-of-mass coordinates), we can express $\boldsymbol{N}$ as a function of the relative position $\boldsymbol{R} = \boldsymbol{r}_0 - \boldsymbol{r}'_0$ of the two bodies; the functional dependence of $\boldsymbol{N}$ on $\boldsymbol{R}$ is determined by the internal geometry of the bodies.

Applying the reciprocity theorem for magnetization [e.g., *Brown*, 1962] to the interaction between these bodies,

$$\int_\tau \boldsymbol{M} \cdot \boldsymbol{H}' d\tau = \int_{\tau'} \boldsymbol{M}' \cdot \boldsymbol{H} d\tau', \tag{10}$$

where $\boldsymbol{H}$ is the field due to $\boldsymbol{M}$ and $\boldsymbol{H}'$ is the field due to $\boldsymbol{M}'$. Assuming the volumes τ and τ' are equal and the magnetization in each volume is uniform, and applying equation (6),

$$\begin{aligned} \boldsymbol{M} \cdot \boldsymbol{N}(\boldsymbol{R}) \cdot \boldsymbol{M}' &= \boldsymbol{M}' \cdot \boldsymbol{N}(-\boldsymbol{R}) \cdot \boldsymbol{M} \\ &= \boldsymbol{M} \cdot \boldsymbol{N}(-\boldsymbol{R}) \cdot \boldsymbol{M}' \end{aligned} \tag{11}$$

(since $\boldsymbol{N}$ is symmetric), so $\boldsymbol{N}(\boldsymbol{R}) = \boldsymbol{N}(-\boldsymbol{R})$.

The volume integrals in equation (7) can be reduced to surface integrals using a version of Gauss's theorem [*Arfken*, 1985]:

$$\begin{aligned} \boldsymbol{N} &= \frac{1}{4\pi\tau} \int_\tau d\tau \nabla \int_{\tau'} \nabla' \left(\frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|}\right) d\tau' \\ &= \frac{1}{4\pi\tau} \int_S d\boldsymbol{S} \int_{S'} \frac{d\boldsymbol{S}'}{|\boldsymbol{r} - \boldsymbol{r}'|}. \end{aligned} \tag{12}$$

Here $d\boldsymbol{S} = \hat{\boldsymbol{n}} dS$, where $\hat{\boldsymbol{n}}$ is the normal to the surface. For example, the component N_{xx} would be obtained by replacing $d\boldsymbol{S}$ by $n_x dy dz$ and $d\boldsymbol{S}'$ by $n'_x dy' dz'$. Later, we will consider a case where all the surfaces are planar surfaces, which simplifies the calculations considerably, but equation (12) is applicable to any pair of continuous, closed surfaces.

Demagnetizing Tensor for a Sphere

It is instructive to consider $\boldsymbol{N}$ for a sphere with volume τ and magnetization $\boldsymbol{M}$. Outside a sphere, the field is the same as that of a point dipole at the center of the sphere. This case is of particular interest because the field due to any finite magnetic body looks like a dipole field sufficiently far away [*Jackson*, 1975].

The field is given by

$$\boldsymbol{H} = \frac{3\boldsymbol{R}(\boldsymbol{m} \cdot \boldsymbol{R}) - \boldsymbol{m} R^2}{4\pi R^5}, \tag{13}$$

where $\boldsymbol{m} = \tau \boldsymbol{M}$ is the total magnetic moment of the sphere.

Writing the components of $\boldsymbol{H}$ explicitly,

$$\begin{aligned} H_x &= \frac{\tau}{4\pi R^5}[M_x(2X^2 - Y^2 - Z^2) + 3M_y XY + 3M_z XZ] \\ H_y &= \frac{\tau}{4\pi R^5}[3M_x XY + M_y(2Y^2 - X^2 - Z^2) + 3M_z YZ] \\ H_z &= \frac{\tau}{4\pi R^5}[3M_x XZ + 3M_y YZ + M_z(2Z^2 - X^2 - Y^2)], \end{aligned} \tag{14}$$

Thus the demagnetizing tensor is given by

$$\boldsymbol{N}(X,Y,Z) = -\frac{3\tau}{4\pi R^5} \begin{bmatrix} X^2 - R^2/3 & XY & XZ \\ XY & Y^2 - R^2/3 & YZ \\ XZ & YZ & Z^2 - R^2/3 \end{bmatrix} \tag{15}$$

The self-demagnetizing tensor is even simpler. Inside a uniformly magnetized sphere, $\boldsymbol{H} = -\boldsymbol{M}/3$, so $\boldsymbol{N} = \boldsymbol{1}/3$, where $\boldsymbol{1}$ is the identity. This is also true of a uniformly magnetized cube, since $N_{xx} = N_{yy} = N_{zz}$ by symmetry and the trace is 1.

Application to Nonuniform Magnetization

The macroscopic fields which appear in Maxwell's equations for media are spatial averages of microscopic fields over volumes large compared to lattice spacing. The microscopic fields involve quantum effects and fluctuate rapidly in time and space. Spatial averaging of these fields results in functions which are fairly smooth, and the averaging can be rigorously justified [e.g., *Jackson*, 1975, section 6.7]. Thus in micromagnetics it is entirely appropriate to represent the magnetization or magnetic field at a point by the average for a region around that point.

Let the magnetization be represented by a discrete distribution $\{\boldsymbol{M}_i\}$ of fields at points $\{\boldsymbol{r}_i\}$. The field at $\boldsymbol{r}_i$ is then

$$\boldsymbol{H}_i = -\sum_j \boldsymbol{N}(\boldsymbol{r}_i - \boldsymbol{r}_j) \cdot \boldsymbol{M}_j, \tag{16}$$

where the sum is over all points including i. The total demagnetizing energy is

$$E_d = -\frac{\mu_0}{2} \sum_i \boldsymbol{M}_i \cdot \boldsymbol{H}_i \tau_i = \frac{\mu_0}{2} \sum_{ij} \boldsymbol{M}_i \cdot \boldsymbol{N}(\boldsymbol{r}_i - \boldsymbol{r}_j) \cdot \boldsymbol{M}_j \tau_i, \tag{17}$$

where

$$\boldsymbol{N}(\boldsymbol{r}_i - \boldsymbol{r}_j) = \frac{1}{4\pi\tau_i} \int_{S_i} d\boldsymbol{S} \int_{S'_j} \frac{d\boldsymbol{S}'}{|\boldsymbol{r} - \boldsymbol{r}'|}. \tag{18}$$

As pointed out above, the region over which the field is averaged should be large compared to a lattice spacing (but also sufficiently small to resolve features like domain walls). This does not necessarily mean that the macroscopic field is uniform within each region, but it should be a smooth function which fits the points $\{\boldsymbol{H}_i\}$.

It would be a mistake to calculate $\boldsymbol{H} = -\nabla\Phi_M$

from equation (4) (without averaging). This function would have small-scale variations unrelated to real field variations, due to the fact that the magnetization is treated as discrete.

Application to an Array of Rectangular Blocks

We now consider a model which divides a ferromagnet into rectangular blocks which have dimensions $\Delta x, \Delta y$ and Δz in the x, y and z directions, respectively. A specialized version of this model for $\Delta x = \Delta y = \Delta z$ was used by *Williams and Dunlop* [1989]; a two-dimensional version with the moment depending only on x and y and $\Delta x = \Delta y \neq \Delta z$ is given in the companion paper [*Newell et al.*, this issue].

Let us consider two such blocks (Figure 1). The coordinates (x, y, z) and (x', y', z') within each block are referred to one corner of the block, and the relative position (X, Y, Z) of the two blocks is the vector between the reference points.

Each component of the demagnetizing tensor involves interactions between two pairs of rectangular surfaces. For example, if we wish to calculate N_{xx} in the manner described after equation (12), we need only consider the two yz faces in each block (Figure 1a), since the normals to the other faces have no component in the x direction. Similarly, N_{xy} is the sum of integrals involving the yz faces in the first block and the xz faces in the second block (Figure 1b). All the other components of N can be obtained from N_{xx} and N_{xy} by permuting the variables. We consider these two cases below.

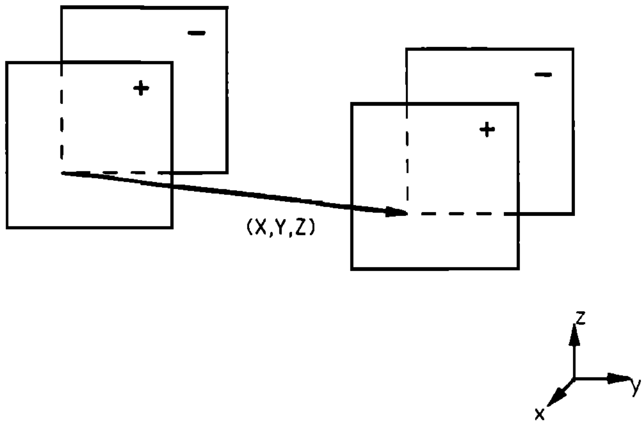

Fig. 1a. The surfaces involved in the component N_{xx}. The signs indicate the direction of the outward normal to the surface. In the integral, the interaction of two surfaces of the same polarity contribute a positive quantity; two surfaces of opposite polarity contribute a negative term (see equation (16)).

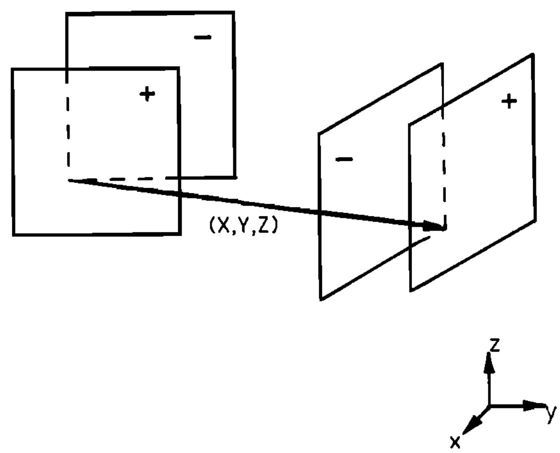

Fig. 1b. The surfaces involved in the component N_{xy}.

Component N_{xx}

The cells have reflection symmetry about three planes. It is easy to see by considering Figure 1a that N_{xx} is even in X, Y and Z. We can separate N_{xx} into four interactions between parallel faces:

$$N_{xx}(X,Y,Z) = \frac{1}{4\pi\tau}\left[2F(X,Y,Z) - F(X+\Delta x,Y,Z) - F(X-\Delta x,Y,Z)\right], \tag{19}$$

where $\tau = \Delta x \Delta y \Delta z$ and the negative signs come from interactions between faces with opposite signs;

$$F(X,Y,Z) = \int_0^{\Delta z}\int_0^{\Delta y}\int_0^{\Delta z}\int_0^{\Delta y} \frac{dz\,dy\,dz'\,dy'}{\sqrt{X^2 + (y+Y-y')^2 + (z+Z-z')^2}}. \tag{20}$$

Note that N_{xx} and F are dependent implicitly on Δy and Δz. When this integral is calculated, care must be taken with the sign of the terms which are being squared. If η is one of the four variables in the integrand, the integrand for the first integration can be written as $f(\eta) = 1/\sqrt{\eta^2 + a^2}$, where a is a constant. But the integral of $f(\eta)$ has two branches:

$$\begin{aligned}\int f(\eta)d\eta &= \ln(\sqrt{\eta^2+a^2}+\eta), \eta > 0 \\ &= -\ln(\sqrt{\eta^2+a^2}-\eta), \eta < 0.\end{aligned} \tag{21}$$

Note that $\ln(\sqrt{\eta^2+a^2}+\eta) + \ln(\sqrt{\eta^2+a^2}-\eta) = 2\ln a$, so the two branches differ by a constant. If, however, $a = 0$, the wrong branch will be divergent. In any case, three more integrations will introduce spurious variables. This mistake is made by *Schabes and Aharoni* [1987].

We will make sure that the quantities which are being squared are always positive. This problem has already been worked out by *Rhodes and Rowlands* [1954]. The integral (20) can be rewritten

$$F(X,Y,Z) = \int_Z^{Z+\Delta z}\int_Y^{Y+\Delta y}\int_{z-\Delta z}^{z}\int_{y-\Delta y}^{y} \frac{dz\ dy\ dz'\ dy'}{\sqrt{X^2+y'^2+z'^2}}. \tag{22}$$

This can be split up into sixteen integrals of the form

$$F_2(X,Y,Z) = \int_0^Z\int_0^Y\int_0^z\int_0^y \frac{dz\ dy\ dz'\ dy'}{\sqrt{X^2+y'^2+z'^2}}. \tag{23}$$

Taking advantage of the fact that this integral is even in Y and Z, we can replace Y and Z by their absolute values. It is convenient to split up the integrals into four sets of four:

$$F(X,Y,Z) = F_1(X,Y+\Delta y, Z+\Delta z) - F_1(X,Y,Z+\Delta z) - F_1(X,Y+\Delta y,Z) + F_1(X,Y,Z), \tag{24}$$

where

$$F_1(X,Y,Z) = F_2(X,Y,Z) - F_2(X,Y-\Delta y,Z) - F_2(X,Y,Z-\Delta z) + F_2(X,Y-\Delta y, Z-\Delta z) \tag{25}$$

The function $F_2(X,Y,Z)$ corresponds to the function $F(p,q)$ of *Rhodes and Rowlands* [1954, equation 2.18] as follows: $F_2(X,Y,Z) = (1/2)Z^3F(Y/Z, X/Z)$.

Finally,

$$F_2(X,Y,Z) = f(X,Y,Z) - f(X,0,Z) - f(X,Y,0) + f(X,0,0) \tag{26}$$

where f is the indefinite integral

$$\begin{aligned} f(x,y,z) = {} & (y/2)(z^2-x^2)\phi\left(\frac{y}{\sqrt{x^2+z^2}}\right) \\ & + (z/2)(y^2-x^2)\phi\left(\frac{z}{\sqrt{x^2+y^2}}\right) \\ & - xyz\tan^{-1}\left(\frac{yz}{xR}\right) + (1/6)(2x^2-y^2-z^2)R \end{aligned} \tag{27}$$

where $\phi(x) \equiv \sinh^{-1}(x) \equiv \ln(x+\sqrt{1+x^2})$ and $R = \sqrt{x^2+y^2+z^2}$. Note that the fact that f is even in x,y and z ensures that F_2 is also.

Component N_{xy}

Considering Figure 1*b*, we see that N_{xy} is even in Z and odd in X and Y (in the latter two cases, the roles of a positive and a negative face get reversed). N_{xy} can be written

$$N_{xy}(X,Y,Z) = (1/4\pi\tau)[G(X,Y,Z) - G(X-\Delta x, Y, Z) - G(X, Y+\Delta y, Z) + G(X-\Delta x, Y+\Delta y, Z)] \tag{28}$$

The factor for two faces can be written

$$\begin{aligned} & G(X,Y,Z) \\ & = \int_{Y-\Delta y}^{Y}\int_{Z-\Delta z}^{Z}\int_{z}^{z+\Delta z}\int_{X}^{X+\Delta x}\frac{dy\ dz\ dz'\ dx'}{\sqrt{x'^2+y^2+z'^2}} \\ & = G_1(X,Y,Z) - G_1(X,Y-\Delta y,Z) \\ & - G_1(X,Y,Z-\Delta z) + G_1(X,Y-\Delta y, Z-\Delta z) \end{aligned} \tag{29}$$

where

$$G_1(X,Y,Z) = G_2(X+\Delta x, Y, Z+\Delta z) - G_2(X+\Delta x, Y, Z) - G_2(X,Y,Z+\Delta z) + G_2(X,Y,Z) \tag{30}$$

where

$$G_2(x,y,z) = g(x,y,z) - g(x,y,0) \tag{31}$$

and

$$\begin{aligned} g(x,y,z) = {} & (xyz)\sinh^{-1}\left(\frac{z}{\sqrt{x^2+y^2}}\right) \\ & + (y/6)(3z^2-y^2)\sinh^{-1}\left(\frac{x}{\sqrt{y^2+z^2}}\right) \\ & + (x/6)(3z^2-x^2)\sinh^{-1}\left(\frac{y}{\sqrt{x^2+z^2}}\right) \\ & - (z^3/6)\tan^{-1}\left(\frac{xy}{zR}\right) - (zy^2/2)\tan^{-1}\left(\frac{xz}{yR}\right) \\ & - (zx^2/2)\tan^{-1}\left(\frac{yz}{xR}\right) - xyR/3. \end{aligned} \tag{32}$$

Other Components N_{ij}

The diagonal elements of the demagnetizing tensor correspond to interactions where the faces in the second block are parallel to the faces in the first block , while the off-diagonal elements are for interactions between perpendicular faces. Thus all the integrals have the same form as either N_{xx} or N_{xy}. The remaining components can be obtained simply by permuting the variables X, Y, Z and the cell dimensions $\Delta x, \Delta y, \Delta z$. For example, if we show the dependence on cell dimensions explicitly, then $N_{yy}(X,Y,Z,\Delta x,\Delta y,\Delta z) = N_{xx}(Y,X,Z,\Delta y,\Delta x,\Delta z)$.

Practical Advantages for Numerical Models

One advantage of the tensor described in equations (19)-(32) is its great generality. Without change, it can be applied to one-, two-, and three-dimensional micromagnetic models with rectangular cells. It is not difficult to modify it to include the even more general case of two cells with unequal dimensions. Because it is a geometric factor, it can be calculated once and then used repeatedly.

Equally important, a computer implementation of this tensor is easy to test, because of the tensor properties (particularly the fact that the trace is either 0 or 1) and the symmetries described in previous sections. There is even the asymptotic condition that the tensor must converge on the tensor for a sphere (equation (15)) as $R \to \infty$. The importance of these tests becomes apparent if one considers how complicated the magnetostatic integrals are.

There is also the advantage of efficiency. A considerable amount of computation is avoided because the geometrical factors, which are the most complicated part of the expression for the energy, need only be calculated once. In addition, there are many cases where one can take advantage of the symmetry properties described in the previous sections to reduce the number of tensor components which must be calculated.

CONCLUSIONS

In uniformly magnetized ellipsoidal particles, the demagnetizing tensor is a useful concept which expresses the dependence of the magnetic response on the shape of the particle. Numerous attempts [*Dunlop*, 1983, 1984; *Xu and Merrill*, 1987] have been made to derive demagnetizing factors for multidomain (MD) states and relate them to experimentally observed quantities such as the susceptibility χ and the coercivity H_c.

This MD demagnetizing factor has played an important role in rock magnetism. In his theory of thermal remanent magnetization, *Néel* [1955] assumed that there was an average demagnetizing factor for a MD grain. All subsequent thermoremanent magnetization theories for MD particles have made the same assumption, with some qualifications [*Dunlop and Waddington*, 1975; *Merrill*, 1977, 1981]. The authors of these theories have recognized, however, that the demagnetizing field depends on the specific domain configuration. In addition, the demagnetizing field plays a dominant role in determining the domain structure itself.

While this paper does not answer the question of whether an average demagnetizing factor exists, it does at least show that there is a rigorous generalization of the demagnetizing tensor. This generalization separates the geometry of the particle (which remains fixed) from the magnetization (which is varied to obtain a stable configuration). Once the demagnetizing tensors are calculated, they can be used repeatedly for a given particle geometry.

In addition to the advantages of this tensor expression mentioned in the previous section, there is also the fact that one can calculate, simultaneously, the equilibrium magnetization and the demagnetizing field. Since it is the field which is measured in most domain observations, this allows direct comparisons between theory and experiment.

Finally, the generalized demagnetizing tensor may be useful in characterizing the effect of surface irregularities or corners, for example in nucleating new domains. Nucleation theory applied to ellipsoidal particles fails to account for observed hysteresis properties of perfect crystals: for example, the predicted coercivity is much too high. This problem became known as Brown's paradox.

Recently, however, *Hartmann* [1987*b*] showed that the discrepancy is due to the sharp corners in real crystals. It appears that large stray fields in the corners can nucleate domains. This was recognized by *Dunlop et al.* [1990], and the field was calculated for a uniformly magnetized cube. The expression for the field in that paper was far too complicated, however, to allow field calculations for realistic magnetization patterns. In the companion paper, we use the generalized demagnetizing tensor to do just that.

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