

Micromagnetics: Basic Principles

A small class of materials exhibit the important property of long range magnetic order. Fundamentally, this arises because of the so-called “exchange energy” which can, under certain circumstances, lead to parallel alignment of neighboring atomic spins. Given the link between the atomic spin and magnetic moment, the spin order gives rise to the observed long range magnetic order. The origin of the long range magnetic order is a fundamental scientific problem which has been studied extensively, both theoretically and experimentally and is now understood in some depth. However, within magnetism there is a major problem when relating fundamental atomic properties to magnetization structures and magnetization reversal mechanisms in bulk materials.

The problem was described vividly by Aharoni (1996) in his discussion of magnetostatic effects. The essential idea is that the material properties are determined by the exchange energy, which in principle is effective on a length scale of subnanometers, and the magnetostatic energy, which has contribution from the boundaries of the material itself and which introduce a different length scale entirely. The challenge of micromagnetics is to develop a formalism in which the macroscopic properties of a material can be simulated including the best approximations to the fundamental atomic behavior of the material.

In brief, the classical approach to micromagnetics replaces the spin by classical vector field which initially allows the determination of magnetostatic fields within the system. In addition to this a different approach to the exchange interaction much be formulated which can replace the quantum mechanical exchange interaction with a formalism appropriate for the limit of continuous material. This, coupled with an energy minimization approach, forms the basis of classical micromagnetics which will be outlined in a later section.

The history of micromagnetics starts with a 1935 paper of Landau and Lifshitz on the structure of a wall between two antiparallel domains, and several papers by Brown around 1940. A detailed treatment of micromagnetism is given by Brown in his 1963 book (Brown 1963).

For many years micromagnetics was limited to the use of standard energy minimization approaches to determine domain structures and classical nucleation theory to determine magnetization reversal mechanisms in systems with ideal geometry. Arguably, the current interest in micromagnetics arises from the availability, from about the mid-1980s onward, of large-scale computing power which enabled the study of more realistic problems which were more amenable to comparison with experimental data.

One important realization during this period was the fact that energy minimization approaches in

principle only determine nucleation fields for the system, and do not predict necessarily correctly the state of the system after magnetization reversal. Consequently, a lot of work has gone into the development of dynamic approaches which use simulations based on the Landau–Lifshitz equation of motion. This is probably the technique in most common use today.

The other area in which considerable development has taken place during the 1990s is that of the calculation of magnetostatic fields, which because of its complexity forms the largest part of most micromagnetic calculations. A number of techniques are available and it is the intention in this review to outline each technique and give consideration to the circumstances under which each one is most applicable.

1. Energy Terms

1.1 Exchange Energy

Exchange energy forms an important part of the covalent bond of many solids and is also responsible for ferromagnetic coupling. The exchange energy is given by

$$E_{exch} = -2JS_1 \cdot S_2 \quad (1)$$

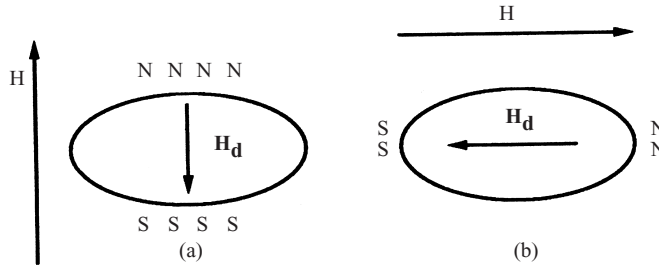
where J is referred to as the exchange integral. S_1 and S_2 are the atomic spins. Clearly for ferromagnetic ordering J must be positive. This so-called direct exchange coupling is somewhat idealized and applicable to only a few materials rigorously.

A number of other models exist, including itinerant electron ferromagnetism and indirect exchange interaction or Ruderman–Kittel–Kasuya–Yoshida (RKKY) interaction. Generally speaking, however, Eqn. (1) is the form usually taken for the exchange interaction with the value of J dependent on the detailed atomic properties of the material.

1.2 Anisotropy

The term anisotropy refers to the fact that the properties of a magnetic material are dependent on the directions in which they are measured. Anisotropy makes an important contribution to hysteresis in magnetic materials and is therefore of considerable practical importance. The anisotropy has a number of possible origins.

(a) *Crystal or magnetocrystalline anisotropy.* This is the only contribution intrinsic to the material. It has its origins at the atomic level. First, in materials with a large anisotropy there is a strong coupling between the spin and orbital angular momenta within an atom. In addition, the atomic orbitals are


Figure 1

Sample with an anisotropic shape with a magnetic field applied in two perpendicular directions: (a) parallel to the short axis; here the “free poles” are separated by a relatively short distance, leading to a large H_d , (b) parallel to the long axis; poles separated by a smaller distance, which leads to a small value of H_d .

generally nonspherical.

Because of their shape the orbits prefer to lie in certain crystallographic directions. The spin-orbit coupling then assures a preferred direction for the magnetization—called the *easy direction*. To rotate the magnetization away from the easy direction costs energy—and *anisotropy energy*. As might be expected the anisotropy energy depends on the lattice structure.

(i) Uniaxial anisotropy occurs in hexagonal crystals such as cobalt.

$$E = KV \sin^2 \theta + \text{higher terms} \quad (2)$$

Here θ is the angle between the easy direction and the magnetization, K is the anisotropy constant, and V the volume of the sample. The higher order terms are small and usually neglected. This has one “easy axis” with two energy minima, separated by energy maxima. This energy barrier leads to hysteresis.

(ii) Cubic anisotropy; for example, iron, nickel

$$E/V = K_0 + K_1 (\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_1^2 \alpha_3^2) \quad (3)$$

Here α gives the direction cosine, i.e., the cosine of the angle between the magnetization direction and the crystal axis.

(b) *Shape anisotropy*. Consider a uniformly magnetized body. By analogy with dielectric materials we can refer to the magnetization (magnetic polarization) creating fictitious “free poles” at the surface.

These lead to a “demagnetizing field” H_d which acts in opposition to \mathbf{H} . Figure 1 shows a sample with an anisotropic shape with a magnetic field applied in two perpendicular directions. The energy increases as H_d increases. For an ellipsoid of revolution it can be shown that

$$E = -K_{eff} V \sin^2 \theta \quad (4)$$

i.e., the same form as for uniaxial anisotropy. θ is the angle between the long axis of the sample and the magnetization direction. Also,

$$K_{eff} = \frac{1}{2}(N_b - N_a) M^2 \quad (5)$$

where \mathbf{M} is the magnetization and N_b and N_a are “demagnetizing factors” in the short axis and long axis directions. N_b and N_a depend on the geometry so that $K_{eff} = 0$ for a sphere and $K_{eff} = M^2/2$ for a needle-like sample.

(c) *Stress anisotropy*. This arises from the change in atomic structures as a material is deformed. It is related to the phenomenon of “magnetostriction” which is important for sensor applications.

(d) *Magnetostatic effects and domain formation*. Magnetostatic fields are a natural consequence arising from any magnetization distribution. The magnetostatic fields are fundamental to the micromagnetic problem and, importantly, introduce another length scale. Magnetostatic effects give rise to magnetization structures on a length scale orders of magnitude greater than atomic spacings. Consequently it is impossible to deal with both magnetostatic and exchange effects rigorously in micromagnetic calculations at least with the current computer facilities. The formulation of the magnetostatic interaction field problem will be given in detail later but for the moment it is simply necessary to introduce the fact that because of magnetostatic fields a magnetized body has a magnetostatic self energy given by

$$E_{mag} = \frac{1}{2} N_a M^2 \quad (6)$$

where N_a is a factor depending on the shape of the sample.

This is, of course, related to the statement (Aharoni 1996) that the energy of a system depends on the boundary of the material. Clearly the energy given by Eqn. (6) can be reduced if the magnetization \mathbf{M} is reduced. As a result of this the material has a tendency to break into domains in which the magnetization remains at the spontaneous magnetization appropriate for a given material at a given temperature with the domains oriented in such a way as to minimize the overall magnetization and hence the magnetostatic self energy.

However, creating a boundary between two domains also requires energy and the actual domain structure depends on a minimization of the total exchange *and* magnetostatic self-energy. This in a sense was the first application of micromagnetics.

It is interesting to note that as the size of a system reduces the magnetostatic self energy reduces and at some point it becomes energetically unfavorable to form a domain structure since the lowering of the magnetostatic energy is not sufficient to compensate for the energy necessary to create the domain wall. Below this size a sample is referred to as single domain and here the magnetization processes are dominated by the rotation of the magnetic moment against the anisotropy energy barrier.

2. Foundations of Micromagnetics

It is not possible to neglect any of the three major energy terms, exchange, anisotropy, and magnetostatic. The detailed magnetic behavior of a given material depends on the detailed balance between these energy terms. It is not even possible to add the magnetostatic and anisotropy terms as a perturbation to the exchange energy term and use a quantum mechanical solution of this problem. Currently the only realistic approach is to ignore the atomic nature of matter, to neglect quantum effects, and to use classical physics in a continuum description of a magnetic material. Essentially, we assume the magnetization to be a continuous vector field $\mathbf{M}(\mathbf{r})$, with \mathbf{r} the position vector. Thus we write

$$\mathbf{M}(\mathbf{r}) = M_s \mathbf{m}(\mathbf{r}); \quad \mathbf{m} \cdot \mathbf{m} = 1 \quad (7)$$

where M_s is the saturation magnetization of the material. The basic micromagnetic approach is to formulate the energy in terms of the continuous magnetization vector field and to minimize this energy in order to determine static magnetization structures. Classical nucleation theory can be used to study modes of magnetization reversal and nucleation fields. The energy terms are formulated as follows.

2.1 Anisotropy Energy

This remains a local calculation and is straightforward to carry out using the expressions for either cubic or uniaxial symmetry given earlier.

2.2 Exchange Energy

The exchange energy is essentially short ranged and involves a summation over the nearest neighbors. Assuming a slowly spatially varying magnetization the exchange energy can be written

$$E_{exch} = JS^2 \sum \phi_{ij}^2 \quad (8)$$

the summation being carried out over nearest neighbors only. The ϕ_{ij} represents the angle between two neighboring spins i and j . It should be noted that in Eqn. (8) the energy of the state in which all spins are aligned has been subtracted and used as a reference state. This is legitimate as long as it is done consistently. For small angles, $|\phi_{ij}| \approx |\mathbf{m}_i - \mathbf{m}_j|$, a first-order expansion in a Taylor series is

$$|\mathbf{m}_i - \mathbf{m}_j| = |(\mathbf{s}_i \cdot \nabla) \mathbf{m}_j| \quad (9)$$

where \mathbf{s} is a position vector joining lattice points i and j .

Substituting, Eqn. (9) into Eqn. (10) gives

$$E_{exch} = JS^2 \sum_i \sum_{s_i} |(\mathbf{s}_i \cdot \nabla) \mathbf{m}_j|^2 \quad (10)$$

where the second summation is over nearest neighbors. Changing the first summation to an integral over the whole body, the result is that for cubic crystals

$$E_{exch} = \int_V W_e dV; \quad W_e = A(\nabla \mathbf{M})^2 \quad (11)$$

where

$$(\nabla \mathbf{M})^2 = (\nabla M_x)^2 + (\nabla M_y)^2 + (\nabla M_z)^2 \quad (12)$$

The material constant $A = JS^2/a$ for a simple cubic lattice with lattice constant a . This represents a major step in the formulation of micromagnetism: we have related the fundamental atomic properties to the spatial derivatives of the magnetization in the continuum approximation. The atomic properties are included via the exchange integral J which in micromagnetic terms is essentially a phenomenological constant which can be determined from experimental data.

2.3 Magnetostatic Fields

Here we consider only the magnetostatic field arising from the magnetization distribution itself and not any externally applied field which is trivial to add to the overall energy. The magnetostatic or demagnetizing field \mathbf{H}_d is governed by Eqns. (13) and (14)

$$\nabla \times \mathbf{H}_d = 0 \quad (13)$$

$$\nabla(\mathbf{H}_d + 4\pi\mathbf{M}) = 0 \quad (14)$$

Eqns. (13) and (14) are written in cgs units, i.e., $\mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}$. Since the curl of \mathbf{H}_d is 0, the demagnetizing field can be derived from a scalar potential,

$$\mathbf{H}_d = -\nabla\phi \quad (15)$$

Substitution of Eqn. (15) into Eqn. (14) yields

$$\nabla^2\phi = -4\pi\nabla \cdot \mathbf{M} \quad (16)$$

which because of its analogy with Poisson's equation in electrostatics leads to the definition of a volume magnetic charge density given by

$$\rho = -4\pi \nabla \cdot \mathbf{M} \quad (17)$$

Thus we can solve for the magnetostatic field by solving for the potential using Eqn. (16) subject to boundary conditions which determine the continuity of the normal component of \mathbf{B} and of the tangential component of \mathbf{H}_d .

$$\mathbf{n} \cdot (\mathbf{B}_{ext} - \mathbf{B}_{int}) = 0 \quad (18)$$

$$\mathbf{n} \times (\mathbf{H}_{d,ext} - \mathbf{H}_{d,int}) = 0 \quad (19)$$

where \mathbf{n} is a unit vector pointing outward from the surface.

In terms of the scalar potential the equivalent conditions are

$$\phi_{ext} = \phi_{int} \quad (20)$$

$$\left. \frac{\partial \phi}{\partial n} \right|_{ext} - \left. \frac{\partial \phi}{\partial n} \right|_{int} = -4\pi \mathbf{M} \cdot \mathbf{n} \quad (21)$$

Thus again the surface of a bulk magnetized body is determining the overall response of a phenomenon having its origins at the atomic level. Finally we can write expressions for the potential and demagnetizing field as follows:

$$\phi(\mathbf{r}) = - \int_V \frac{\nabla \cdot \mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' + \int_S \frac{\mathbf{M}(\mathbf{r}') \cdot \mathbf{n}}{|\mathbf{r} - \mathbf{r}'|} dS' \quad (22)$$

$$\begin{aligned} \mathbf{H}_d = & - \int_V \frac{(\mathbf{r} - \mathbf{r}') \nabla \cdot \mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} dV' \\ & + \int_S \frac{(\mathbf{r} - \mathbf{r}') \mathbf{M}(\mathbf{r}') \cdot \mathbf{n}}{|\mathbf{r} - \mathbf{r}'|^3} dS' \end{aligned} \quad (23)$$

The integrals in Eqn. (23) can be interpreted as fields arising from volume and surface charge densities $\rho = -4\pi \nabla \cdot \mathbf{M}$ and $\sigma = 4\pi \mathbf{M}(\mathbf{r}) \cdot \mathbf{n}$, respectively.

Although Eqns. (22) and (23) represent elegant closed form solutions for the potential and demagnetizing field, they are not the best form for numerical computation. Essentially, the total energy of the system involves an integral over the volume as follows:

$$E_{mag} = \frac{1}{2} \int_V \mathbf{H}_d \cdot \mathbf{M} dV \quad (24)$$

which because of Eqn. (23) involves a six-fold integration. In terms of the numerical problem this involves a scaling with N^2 , where N is the number of elements into which the body is discretized. This of course leads to rapid degradation of computational speed with system size and in practice an alternative solution must be found for the calculation of \mathbf{H}_d . The techniques involved will be described in detail later.

2.4 Brown's Equations

The final step in the formulation of classical micromagnetics is to minimize the total energy which can be written as follows

$$E_{tot} = \int_V \left[A(\nabla \mathbf{M})^2 + E_{anis} - M_s \mathbf{m} \cdot \left(\mathbf{H}_a + \frac{\mathbf{H}_d}{2} \right) \right] dV \quad (25)$$

where \mathbf{H}_a is the externally applied field. Here, E_{anis} is the anisotropy energy density.

The approach uses standard variational principles but the derivation is somewhat protracted. Essentially, setting the first variation of the total energy to zero leads to two equations. The first is a surface equation

$$2A \left[\mathbf{m} \times \frac{\partial \mathbf{m}}{\partial n} \right] = 0 \Rightarrow \frac{\partial \mathbf{m}}{\partial n} = 0 \quad (26)$$

since $\mathbf{m} \cdot \partial \mathbf{m} / \partial n = 0$ by virtue of $\mathbf{m} \cdot \mathbf{m} = 1$. The second is a volume equation,

$$\mathbf{m} \times \left[\frac{2A}{M_s} \nabla^2 \mathbf{m} + \mathbf{H}_d + \mathbf{H}_a + \mathbf{H}_K \right] = 0 \quad (27)$$

where the anisotropy field \mathbf{H}_K is defined as

$$\mathbf{H}_K = - \frac{1}{M_s} \frac{\partial E_{anis}}{\partial \mathbf{m}} \quad (28)$$

Eqn. (27) can be written

$$\mathbf{m} \times \mathbf{H}_{eff} = 0 \quad (29)$$

where the effective field \mathbf{H}_{eff} is

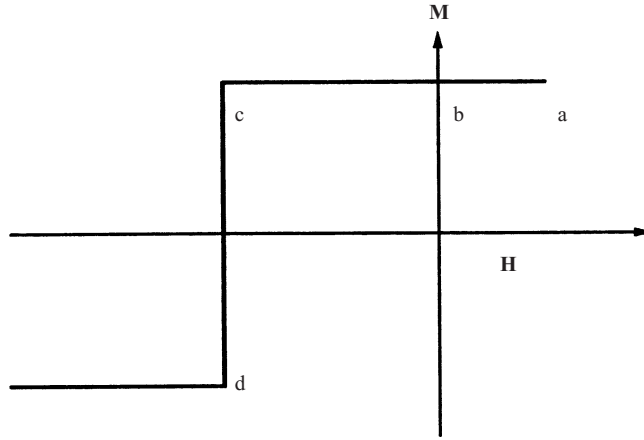
$$\mathbf{H}_{eff} = \frac{2A}{M_s} \nabla^2 \mathbf{m} + \mathbf{H}_d + \mathbf{H}_a + \mathbf{H}_K \quad (30)$$

Eqn. (27) states that the equilibrium solution is found by making the magnetization lie parallel to the local field. Eqns. (26)–(30) are referred to as Brown's equations and form the basis of the classical micromagnetic approach for the solution of stationary problems.

3. Analytical Solutions

3.1 Stoner–Wohlfarth Theory

Stoner–Wohlfarth (SW) theory is the simplest micromagnetic model since it is assumed that all spins remain collinear thus removing the exchange term. Consider a particle with uniaxial anisotropy and easy axis at some angle ψ to the applied field. The magnetization of the particle has an angle θ to the easy axis and $\theta - \psi$ to the applied field. The magnetic moment of the particle is MV , where V is the particle


Figure 2

Hysteresis loop for a SW particle with the field applied parallel to the easy axis.

volume. Assuming that the atomic magnetic moments always remain parallel (coherent rotation) the energy is the sum of the anisotropy and field energies, i.e.,

$$E = KV \sin^2 \theta - MVH \cos(\theta - \psi) \quad (31)$$

The orientation of the magnetic moment is determined by minimizing the energy E , that is we set $dE/d\theta = 0$. This gives

$$\frac{dE}{d\theta} = 2KV \sin \theta \cos \theta + MVH \sin(\theta - \psi) = 0 \quad (32)$$

In general there are four solutions of Eqn. (32), two minima and two maxima (which separate the minima). We can illustrate the behavior using the special case of $\psi = 0$, that is, the easy axis is aligned with the field. Then Eqn. (32) becomes

$$2KV \sin \theta \cos \theta + MVH \sin \theta = 0 \quad (33)$$

Eqn. (33) has a solution at $\sin \theta = 0$, i.e., $\theta = 0$ or π . Further solutions occur at $2KV \cos \theta = -MVH$, so that

$$\cos \theta = -MH/2K \quad (34)$$

which are maxima.

These results can be used to illustrate the reversal process in the following way using Fig. 2. A large positive field is first applied to the sample, taking it to point (a) on the hysteresis loop. When the field is reduced to zero the energy maximum stops the system from becoming demagnetized. The magnetization still lies along the easy direction, i.e., in this case parallel to the applied field. This gives a remanent magnetization (point b). In negative fields the magnetization would prefer to reverse, in order to be parallel to the field direction. In order to do this it would have to rotate

over the maximum energy, E_{max} . Thus there is an energy barrier to rotation, of value $E_b = E_{max} - E_{min}$. It is straightforward to show that

$$\begin{aligned} E_b &= KV \left(1 - \frac{M^2 H^2}{4K^2} \right) - MVH \left(\frac{MH}{2K} \right) - (-MVH) \\ &= KV \left(1 + \frac{M^2 H^2}{4K^2} \right) \end{aligned} \quad (35)$$

Therefore, the energy barrier becomes zero when $(MH/2K) = 1$, that is, when $H = -2K/M = -H_K$.

At this point, the *coercive force*, the magnetization rotates into the other minimum, i.e., into the field direction (points c to d). Thus H_K is the maximum coercive force for a particle. For a particle oriented at some angle ψ the behavior consists of a mixture of reversible and irreversible rotation.

The coercive force at some angle ψ is less than H_K . For a system of particles with randomly orientated easy axes an average over all orientations gives a hysteresis loop that has a remanence of half the saturation magnetization and a coercivity of $0.479H_K$.

The SW model is still extensively used, especially in materials where the long-range interaction effects are more important than intrinsic grain properties. Generally, agreement with experiment is obtained for a low "effective value" of H_K which takes some account of the nonuniform magnetization processes as is discussed later in relation to thin film simulations.

3.2 The Nucleation Problem

Consider a ferromagnetic body in a magnetic field large enough to cause saturation. The field is slowly reduced to zero and then increased in a negative sense. At some point the original state becomes unstable and the magnetization makes a transition to a new energy

minimum. The field at which the state becomes unstable is the “nucleation field.” This can be determined analytically for a few simple geometries. In a sense, SW is the simplest nucleation theory. The limitations of nucleation theory can be seen by considering the final state after transition.

In a complex system there may be more than one accessible minimum, rather than the one state of SW theory. Consequently, nucleation theory cannot predict the magnetization curve of anything but the simplest materials and in this sense its predictions are more mathematically than physically interesting. Numerical micromagnetics with its novel techniques for determining the magnetic state at any point of the hysteresis loop is where predictions become accessible to experimental verification.

4. Numerical Micromagnetics

4.1 Calculation of Stationary States: Energy Minimization Versus Dynamic Approach

The first numerical micromagnetic approaches following the resurgence of interest in micromagnetic calculations in the mid-1980s were based essentially on energy minimization. Della Torre (1985, 1986) uses this approach in some calculations on the behavior of elongated particles. The approach works reasonably well but is prone to numerical instabilities.

A more sophisticated minimization technique was developed by Hughes (1983) in studies of longitudinal thin film media consisting of strongly coupled spherical grains (the strong coupling arising from exchange interactions between grains). In these materials strong cooperative reversal is important and a straightforward energy minimization technique was problematic during the magnetization reversal process.

A number of sophisticated energy minimization approaches are possible using standard numerical techniques. For example a number of workers have used conjugate gradient techniques. However, the basic problem arises from the nature of the micromagnetic problem itself. Essentially, it is relatively easy to track a well-defined energy minimum as it evolves with the magnetic field. This is usually the case, for example, in the decrease from magnetic saturation towards the remanent state where no irreversible behavior occurs. The energy minimum in which the system resides is essentially a local energy minimum on a very complex energy surface. The magnetization reversal process can be seen as the disappearance of the local energy minimum due to the action of a sufficiently large field applied in a sense opposite to the original “positive” saturation direction.

The magnetization reversal process takes place when the minimum in the positive field direction vanishes and the system makes a transition into an energy minimum closer to the negative field direction.

If the energy surface has a complex topology it may contain a number of energy minima accessible during the magnetization reversal process. Energy minimization is a very poor technique for predicting the correct minimum.

Magnetization reversal is intrinsically a dynamic phenomenon and in order to predict magnetization states correctly after reversal we should in principle take account of the dynamic behavior of the system as far as is possible. Victora (1987) first used a dynamic approach in studies of longitudinal thin films. The approach is based on the Landau–Lifshitz (L–L) equation of motion of an individual spin, which has the form

$$\frac{d\mathbf{M}}{dt} = \gamma_0 \mathbf{M} \times \mathbf{H} - \frac{\alpha \gamma_0}{M_s} \mathbf{M} \times \mathbf{M} \times \mathbf{H} \quad (36)$$

Here, γ_0 is the gyromagnetic ratio and α is the damping constant. In Eqn. (36) the first term leads to gyromagnetic precession. In the absence of damping this will be eternal and would not lead to the equilibrium state in which the magnetization is parallel to the local field.

The second term represents damping. This ensures that the system eventually reaches the equilibrium position. It should be noted that other forms of the dynamic equation are possible, including the Gilbert form. However, in the limit of small damping, these forms are equivalent although the Gilbert equation is probably more physically correct.

Also, in the limit of large damping, in which case the second term of Eqn. (36) dominates, the Landau–Lifshitz equation is equivalent to a steepest decent energy minimization approach. The L–L equation is the most widely used dynamic approach currently.

Eqn. (36) is easy to solve numerically for a single spin. However, the micromagnetic problem is represented by a set of strongly coupled equations of motions which is a somewhat more difficult numerical problem. The types of system considered can for convenience be considered as of two types.

(i) Weakly coupled systems. Typical examples here might be a set of grains with uniform magnetization coupled by magnetostatic and perhaps weak exchange interactions. For this type of system a simple numerical technique such as the Runge–Kutta approach with adaptive step size will probably suffice.

(ii) Strongly coupled systems. These examples tend to have strong exchange coupling, for example, in the case of studies of nonuniform magnetization processes in a single grain or a set of strongly exchange coupled grains. In terms of the differential equations the system in this case is referred to as “stiff.” Although Runge–Kutta will still give a solution, the step size tends to become very small and the computational times involved, increasingly long. It is more usual under these circumstances to use an alternative technique, for example, predictor–corrector algorithms.

The numerical technique essentially entails the determination of the local field \mathbf{H} at each point in the system followed by a determination of the small magnetization changes using Eqn. (36). The whole system is updated simultaneously at each time step after which the local field is recomputed and this procedure is carried out until the system evolves into an equilibrium state. Equilibrium can be determined using a number of criteria:

(i) Magnetization changes at a given step below a certain minimum value, and

(ii) Comparison of the direction of the local magnetization and the local field. Essentially the convergence is determined dependent on the maximum value of $\mathbf{M} \times \mathbf{H}$ for the system.

The technique used depends to some extent on the system studied. In a sense this is the easiest part of numerical micromagnetics. A number of numerical techniques are available for the solution of Eqn. (36) and it is not too difficult to create algorithms based on the dynamic approach which are robust in terms of finding stationary states and also reliable in finding new stationary states after the nucleation of a magnetization reversal event.

Two problems remain however. The first is the determination of the local field \mathbf{H} which is a rather difficult and specific problem on which considerable effort has been expended. However, a further problem is in the microstructure of the material itself and the approximations which need to be made in order to make the problem amenable to a numerical solution whilst retaining some physical realism. The following section considers some aspects of the problem of microstructure in micromagnetics.

4.2 Microstructural Simulations

Numerical micromagnetics involves a discretization of space. The behavior of the spin associated with each small volume element is described by Eqn. (36). Because of the exchange and magnetostatic interactions this leads to a finite set of coupled equations of motion of the form of Eqn. (36) which have to be solved numerically. The spatial discretization is an important part of the problem.

(a) *Particulate systems.* Nanostructured particulate systems are essentially of two types. The first is so-called granular magnetic solid, essentially a heterogeneous alloy consisting of magnetic particles in a non-magnetic matrix. This is often produced by sputtering, evaporation, or laser ablation. These systems have a microstructure consisting of relatively randomly distributed grains and can be modeled by placing grains at random into the computational cell. The spatial disorder in this system has been shown (El Hilo *et al.* 1994) to be an important factor in deter-

mining the effects of exchange coupling in the materials.

For example, standard micromagnetic calculations with an ordered system lead to an enhancement of the remanent magnetization due to intergranular exchange coupling but also predict a decreased coercive force due to the effects of cooperative magnetization reversal. In a system with a random microstructure, however, the effects of the cooperative reversal are decreased and although the exchange coupling leads to an enhanced remanence the reduction in the scale of the cooperative reversal can also lead to a small enhancement of the coercive force. Consequently, it is important to stress that the microstructure of a material needs to be modeled as realistically as possible.

In the case of particular materials produced by the solidification of a fluid precursor, for example, by the polymerization of a ferrofluid or the production of particulate recording medium from a magnetic dispersion, it is known that magnetostatic interactions are important because they give rise to flux closure and consequent modifications to the microstructure.

Vos *et al.* (1993) have demonstrated the importance of microstructure by comparing the chaining effects which occur in standard particulate media with the behavior of barium ferrite. In the latter case the particles consist of small platelets which tend to form long stacks under the influence of magnetostatic interactions. The calculations of Vos *et al.* indicate very different behavior for the two types of microstructure. However, the actual microstructures used were created using an *ad hoc* procedure.

Chantrell *et al.* (1996) have demonstrated the importance of the correct simulation of microstructure in particulate systems, and have developed a sophisticated molecular dynamic approach Coverdale *et al.* 2001 to the prediction of microstructures.

(b) *Granular thin metallic films.* Although these are similar to particulate materials in that they consist of well-defined grains, these materials are generally considered as a separate case, essentially because of their different applications and also because they consist, to a first approximation at least, as a single layer of grains.

In these systems, clearly magnetostatic interactions between the metallic grains will be very strong and there is also the possibility of some exchange coupling across grain boundaries. Generally these materials are alloys, for example, of chromium. The intention is that the chromium segregates to grain boundaries giving rise to good magnetic isolation.

The first models of these materials were produced from the mid-1980s onwards and in many ways remain largely unchanged. The models consist of spherical grains which are assumed to rotate coherently and can therefore be treated as a single spin,

situated on a regular hexagonal lattice. The reason for this uniformity is that it simplifies the magnetostatic field calculation because fast Fourier transform techniques can be used (as described in the following section).

Many simulations still use this rather idealized model, even though it has been shown that it drastically overestimates the cooperative reversal. Miles and Middleton (1990) were the first to develop a simulation based on an irregular grain structure with a distribution of particle volumes. This and later work (Walmsley *et al.* 1996) demonstrate conclusively that the size of magnetic features in the materials is critically affected by the microstructure and, as one might expect, is significantly smaller in materials with some disorder.

The other problem with the assumed microstructure is the intrinsic assumption of coherent reversal, which means that the intrinsic coercivity (assumed to be due to coherent rotations) is probably overestimated.

The parameters h_{int} and C^* represent the magnetostatic and exchange coupling strengths with respect to the intrinsic coercivity and are empirical parameters which essentially hide the micromagnetic deficiencies of the model. At attempt to produce a realistic microstructure is described by Schrefl and Fidler (1992). The microstructure is produced via a voronoi construction. Essentially this entails, for a two-dimensional system at least, distributing points at random in space and bisecting the line between points to produce grain boundaries. This produces an irregular grain structure and has been used in granular three-dimensional systems (Schrefl and Fidler 1992) and longitudinal thin films (Tako *et al.* 1996).

These models represent the state of the art in terms of microstructural simulations. It is desirable to carry out a discretization of the systems at the subgrain level, since this allows the correct simulation of nonuniform magnetization processes. The uniform mesh is no longer appropriate. Finite element methods are necessary, and are outlined in *Micromagnetics: Finite Element Approach*.

5. Magnetostatic Field Calculations

Here we consider relatively common and easily applied approaches. More sophisticated techniques are necessary for calculations using finite elements, and these will be outlined in *Micromagnetics: Finite Element Approach*.

5.1 Dipole Sum—the Bethe–Peierls–Weiss Approximation

This is by far the easiest approach to adopt. We start with the interaction field written as

$$\mathbf{H}_i = \sum_{j \neq i} \mathbf{H}_{ij} \quad (37)$$

where

$$\mathbf{H}_{ij} = -\frac{\mathbf{m}_j}{r^3} + \frac{3(\mathbf{m}_j \cdot \mathbf{r})\mathbf{r}}{r^5}$$

is the interaction field at element i due to element j . \mathbf{m}_i and \mathbf{m}_j are the magnetic moments of each element and \mathbf{r} is the spatial separation.

Clearly the determination of fields via Eqn. (37) is an N^2 problem. In order to make the calculation feasible for large systems the usual approximation is to divide the problem into a direct summation over some region V around a given site i and to use a continuum approximation to the field outside this region. For a spherical cut off the result is of the form (in cgs units)

$$\mathbf{H}_i = \sum_{j \in V} \mathbf{H}_{ij} + \frac{4\mathbf{M}}{3} - N_a \mathbf{M} \quad (38)$$

The first term is a direct summation within a region V surrounding i . Outside this region the material is treated as a uniformly magnetized continuous material of magnetization \mathbf{M} (in cgs units). The problem of determining the field at the center of the spherical cut out than reduces to solutions of

$$\mathbf{H}_a = \int_{\partial V} \frac{(\mathbf{r}-\mathbf{r}') \cdot \mathbf{M}(\mathbf{r}')\hat{\mathbf{n}}}{|\mathbf{r}-\mathbf{r}'|^3} dS \quad (39)$$

over surfaces ∂V representing the inside surface of the cut out region and the outside of the magnetized body. Eqn. (39) follows directly from Eqn. (23) given the assumption of a uniform magnetization, $\nabla \cdot \mathbf{M} = 0$.

The second and third terms in Eqn. (38) are the ‘‘Lorentz’’ and ‘‘demagnetizing’’ fields arising from the internal and external surfaces respectively, with N_a a shape-dependent demagnetizing factor. These factors arise directly from analytical solution of Eqn. (39).

5.2 Hierarchical Calculation

The hierarchical approach is a more sophisticated calculation which improves on the Bethe–Peierls–Weiss approximation. Essentially, a dipole sum is again carried out within a central area around the point at which the field is to be calculated. In the simplest case the remaining material is represented by ‘‘cells’’ of similar size, taken as having a total moment obtained by adding all the moments in the cell. This is then used to calculate the field due to the cell at the central point and a summation of these contributions is taken. This approach was used by Miles and Middleton (1991). It is possible to improve the accuracy by adding higher order (multipole) terms. Such fast multipole methods are often used in electrostatic calculations.

The beauty of the hierarchical calculation is that it can be applied to systems with disordered microstructures which is not easily the case for methods such as the fast Fourier transform, a description of which follows.

5.3 Fast Fourier Transform Techniques

This was developed by Mansuripur and Giles (Mansuripur and Giles 1988, Giles *et al.* 1990) specifically for simulation of magneto-optic recording media and has since become widely used. Its advantage is that the use of FFTs give rise to a scaling with $M \ln N$ rather than N^2 . The disadvantage is the need for a lattice in order to carry out the discrete Fourier transform. The problem can be formulated in a general way using the following three-dimensional representation formulas:

$$\mathbf{M}(\mathbf{x}) = \sum_{pqr} \mathbf{m}_{pqr} e^{i(\mathbf{k}_{pqr} \cdot \mathbf{x})} \quad (40)$$

$$\phi(\mathbf{x}) = \sum_{pqr} \psi_{pqr} e^{i(\mathbf{k}_{pqr} \cdot \mathbf{x})} \quad (41)$$

Here, $\mathbf{k}_{pqr} = (k_p, k_q, k_r)$ with $k_p = 2\pi p/L_x$, $k_q = 2\pi q/L_y$, $k_r = 2\pi r/L_z$. By substitution into Eqn. (16) and comparing coefficients it is straightforward to show that

$$\phi_{pqr} = -\frac{4\pi i}{|\mathbf{k}_{pqr}|^2} \mathbf{m}_{pqr} \cdot \mathbf{k}_{pqr} \quad (42)$$

Determination of $-\nabla\phi$ then gives the field value.

See also: Micromagnetics: Finite Element Approach; Magnetic Anisotropy; Coercivity Mechanisms; Magnetic Hysteresis

Bibliography

Aharoni A 1996 *Introduction to the Theory of Ferromagnetism*. Clarendon Press, Oxford

- Brown Jr. W F 1963 *Micromagnetics*. Interscience, New York
- Chantrell R W, Coverdale G N, El-Hilo M, O'Grady K 1996 Modelling of interaction effects in fine particle systems. *J. Magn. Magn. Mater.* **157/158**, 250–5
- Coverdale G N, Chantrell K W, Veitch K J 2001 *J. Appl. Phys.* in press
- Della Torre E 1985 Fine particle micromagnetics. *IEEE Trans. Magn.* **21**, 1423–25
- Della Torre E 1986 Magnetization calculation of fine particles. *IEEE Trans. Magn.* **22**, 484–9
- El-Hilo M, O'Grady K, Chantrell K W 1994 The effect of interactions on GMR in granular solids. *J. Appl. Phys.* **76**, 6811–13
- Giles K C, Kotiuga P K, Humphrey F B 1990 Three-dimensional micromagnetic simulations on the connection machine. *J. Appl. Phys.* **67**, 5821–3
- Hughes G F 1983 Magnetization reversal in cobalt-phosphorous films. *J. Appl. Phys.* **54**, 5306–13
- Mansuripur M, Giles K 1988 Demagnetizing field computation for dynamic simulation of the magnetization reversal process. *IEEE Trans. Magn.* **24**, 2326–8
- Miles J J, Middleton B K 1990 The role of microstructure in micromagnetic models of longitudinal thin film magnetic media. *IEEE Trans. Magn.* **26**, 2137–39
- Miles J J, Middleton B K 1991 A hierarchical model of longitudinal thin film recording media. *J. Magn. Magn. Mater.* **95**, 99–108
- Schrefl T, Fidler J 1992 Numerical simulation of magnetization reversal in hard magnetic materials using a finite element method. *J. Magn. Magn. Mater.* **111**, 105–14
- Tako K M, Wongsam M, Chantrell K W 1996 Micromagnetics of polycrystalline two-dimensional platelets. *J. Appl. Phys.* **79**, 5767–9
- Victoria R 1987 Quantitative theory for hysteretic phenomena in CoNi magnetic thin films. *Phys. Rev. Lett.* **58**, 1788
- Vos M J, Brott R L, Zhu J G, Carlson L W 1993 Computed hysteresis behaviour and interaction effects in spheroidal particle assemblies. *IEEE Trans. Magn.* **29**, 3652–7
- Walmsley N S, Hart A, Parker D A, Chantrell R W, Miles J J 1996 A simulation of the role of physical microstructure on feature sizes in exchange coupled longitudinal thin films. *J. Magn. Magn. Mater.* **155**, 28–30

J. Fidler, R. W. Chantrell, T. Schrefl, and M. A. Wongsam

Copyright © 2001 Elsevier Science Ltd.

All rights reserved. No part of this publication may be reproduced, stored in any retrieval system or transmitted in any form or by any means: electronic, electrostatic, magnetic tape, mechanical, photocopying, recording or otherwise, without permission in writing from the publishers.

Encyclopedia of Materials: Science and Technology
ISBN: 0-08-0431526
pp. 5642–5651