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Micromagnetic modeling and analysis for memory and processing applications

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University of California, San Diego

2012
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Micromagnetic Modeling and Analysis for Memory and Processing Applications

by

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Magnetic nanostructures are vital components of numerous existing and prospective magnetic devices, including hard disk drives, magnetic sensors, and microwave generators. The ability to examine and predict the behavior of magnetic nanostructures is essential for improving existing devices and exploring new technologies and areas of application.

This thesis consists of three parts. In part I, key concepts of magnetism are covered (chapter 1), followed by an introduction to micromagnetics (chapter 2). Key interactions are discussed. The Landau-Lifshitz-Gilbert equation is introduced, and the variational approach of W. F. Brown is presented.

Part II is devoted to computational micromagnetics. Interaction energies, fields
and torques, introduced in part I, are transcribed from the continuum to their finite element form. The validity of developed models is discussed with reference to physical assumptions and discretization criteria. Chapter 3 introduces finite element modeling, and provides derivations of micromagnetic fields in the linear basis representation. Spin transfer torques are modeled in chapter 4. Thermal effects are included in the computational framework in chapter 5. Chapter 6 discusses an implementation of the nudged elastic band method for the computation of energy barriers. A model accounting for polycrystallinity is developed in chapter 7. The model takes into account the wide variety of distributions and imperfections which characterize true systems. The modeling presented in chapters 3–7 forms a general framework for the computational study of diverse magnetic phenomena in contemporary structures and devices. Chapter 8 concludes part II with an outline of powerful acceleration schemes, which were essential for the large-scale micromagnetic simulations presented in part III.

Part III begins with the analysis of the perpendicular magnetic recording system (chapter 9). A simulation study of the recording process with readback analysis is presented. Heat-assisted magnetic recording is considered in chapter 10. The effects of optical spot size and switching rate on signal quality are investigated. Chapter 11 is devoted to bit patterned media (BPM). Reversal modes and thermal stability of Co/Pd multilayer islands are studied. A novel BPM design, called capped BPM, is shown to provide enhanced tunability of thermal stability, writability, switching field distributions, and readback. Chapter 12 discusses spin valve applications. An all-perpendicular composite spin valve is shown to significantly reduce the tradeoff between switching currents and thermal stability. The last chapter 13 covers domain wall (DW) devices. DW motion in magnetically frustrated nanorings is analyzed. Antiferromagnetically coupled nanowires are shown to extend DW velocities beyond the Walker breakdown limit. A crosswire architecture is proposed for Boolean operations and the study of disorder dynamics.
Part I

Introduction
1 Magnetism

All materials are magnetic in some form and extent. This is owing to the charge-and angular momentum-bearing particles which constitute materials. Charged particles with angular momentum generate a magnetic moment which produces a magnetic field (Fig. 1.1). Magnetic moments interact with other magnetic moments through their magnetic fields. This is known as the magnetic dipole-dipole interaction, and it is a far-range interaction. As will be discussed shortly, other interaction types exist that couple magnetic moments locally. The response of the net magnetic moment of a material to an externally applied magnetic field depends on how these local magnetic moments are coupled to each other. In copper, glass, and plastic, the net magnetic moment is zero, and the application of a magnetic field does not change the situation appreciably. Hence these materials are called in practice nonmagnetic. Weakly magnetic materials (e.g., iron-bearing minerals, quartz, water) develop a small net moment in the presence of an external magnetic field. In some materials the magnetic moment may orient with the field, in others it may oppose it. Permalloy and other strongly magnetic materials possess a net macroscopic magnetic moment even in the absence of an applied magnetic field. Such magnetic moment is called spontaneous. Magnetism describes the interactions between atomic magnetic moments of a material and their response to an applied magnetic field. We review different types of magnetism and provide some justification for their occurrence in nature.

1.1 Diamagnetism

Diamagnetic materials such as water and diamond are composed of atoms or molecules whose electronic shells are closed, that is, all shell orbitals are occupied by one spin up electron and one spin down electron. A closed (or filled) shell means that the net angular momentum (orbital angular momentum plus spin angular momentum) is zero.
Upon application of a magnetic field, the electron orbitals are distorted, leading to a magnetic moment that opposes the applied field. The response is classically described as a consequence of the Lorenz force, known as Lenz law. The classical description, however, encounters a pitfall in accounting for the conservation of angular momentum, for which quantum mechanics provides the needed remedy [O’Handley, 1999].

The diamagnetic response, as described, does not require necessarily a closed shell for its manifestation. However, it is only closed shell structures where diamagnetism prevails over other forms of magnetism, and therefore, only such systems are called diamagnetic. The susceptibility $\chi$ (unitless), which quantifies the response of the magnetization $M$ (emu/cm$^3$) (magnetic moment density) to an applied magnetic field $H$ (Oe) through the relation $M = \chi H$, thus has a negative value for diamagnetic substances such as water ($-7.2 \times 10^{-7}$), diamond ($-1.7 \times 10^{-6}$), and bismuth ($-1.3 \times 10^{-5}$) (given at $T = 293$ K). The quoted susceptibilities imply that only a relatively weak magnetization may develop in diamagnetic materials in response to an applied magnetic field. An exception is a superconductor, where macroscopic orbits of electrons are possible, and $\chi = -1/4\pi$, implying that an applied magnetic field $H$ is completely screened out inside the diamagnet by the magnetization, i.e., $B = H + 4\pi M = H + 4\pi \chi H = 0$. The diamagnetic susceptibility is broadly temperature independent since the interaction between the applied magnetic field and electron velocity does not require cooperative or orderly electron behavior that can be disrupted by thermal agitation.
1.2 Paramagnetism

Macroscopically, paramagnetic materials, like diamagnetic materials, possess no spontaneous net magnetic moment. However, unlike diamagnetic materials, paramagnets do possess net magnetic moments on an atomic scale. In paramagnetic substances, atoms, ions, or molecules have only partially filled orbitals, resulting in a local net magnetic moment. Atomic moments in paramagnetic materials are largely uncoupled, each free to point in its own arbitrary direction. Hence, the net magnetic moment approaches zero upon averaging over many atomic moments. The situation changes with the application of an external magnetic field. The lowest energy configuration becomes that in which all free moments point in the direction of the applied field. Since the magnetic field can only generate precession of magnetic moments about the field axis, and can do no work in changing the energy, it is the action of the thermal surroundings that assists in the realization of a net macroscopic magnetic moment in paramagnets. The equilibrium net macroscopic moment consists of an ensemble of uncoupled atomic moments biased in the direction of the applied field. The distribution of atomic magnetic moment directions can be deduced from statistical mechanics, and depends on the level of disorder, or temperature. The Curie law states that the paramagnetic susceptibility is inversely proportional to temperature, i.e., \( \chi \propto 1/T \). In the standard model, valid for many paramagnets, the susceptibility is field independent when the applied field is weak (\( H \approx 0 \)); hence the linear relation holds \( M = \chi H \), where \( \chi = C/T \), and \( C \) (K) is the Curie constant. In paramagnetic materials, the paramagnetic response is usually much stronger than the diamagnetic response, resulting in a net positive (paramagnetic) susceptibility, which for oxygen gas is \( 1.5 \times 10^{-7} \), for aluminum \( 1.8 \times 10^{-6} \), and iron oxide \( 5.7 \times 10^{-4} \) (quoted at \( T = 293 \) K).

1.3 Ferromagnetism

Materials dearest to the focus of the present dissertation are ferromagnetic in nature, and, as such, bear a spontaneous macroscopic magnetic moment, meaning that the magnetic moment persists macroscopically even at zero magnetic field. The magnetic moment density of most ferromagnets is very high. Some ferromagnets are permanent or highly incoercible, others can be magnetically soft, a number are preciously magnetoresistive and magnetostrictive, and all are hysteretic, with incremental susceptibilities that
can range in the \(\sim (100–1000)\). The usefulness of such strongly magnetic substances is great. Applications range from electric motors, sensors in automotive systems, and audio speakers to particle accelerators, stealth coating, energy harvesting, magnetic resonance imaging, targeted drug and gene delivery, and finally applications at the heart of this thesis, magnetic recording and information processing.

The spontaneous macroscopic magnetic moment in ferromagnetic materials is a result of the cooperative behavior of neighboring electron spins. This cooperative behavior is a consequence of the Coulomb interaction and the symmetry principle (or quantum state symmetry) by which the wavefunction for a system of indistinguishable fermions must be antisymmetric under particle interchange. The Pauli exclusion principle, widely quoted in describing ferromagnetism, is embodied in the symmetry principle. This is seen by observing the effect of particle interchange of two electrons presumed to be in the same quantum state: \((r_1, r_2) \overset{\text{interchange}}{\rightarrow} (r_2, r_1)\). If the two electrons are indistinguishable and have the same quantum state, one would have that \(\Psi(r_1, r_2) = \Psi(r_2, r_1)\). Due to the principally mediated antisymmetry of the total wavefunction, we must also have that \(\Psi(r_1, r_2) = -\Psi(r_2, r_1)\). The previous two equations imply that \(\Psi(r_1, r_2) = -\Psi(r_1, r_2)\), a condition satisfied only for \(\Psi(r_1, r_2) = 0\). This attests Pauli’s exclusion principle, that the probability of two electrons (or any two indistinguishable fermions) to occupy the same state is precisely zero.

Before considering spontaneous magnetization in bulk ferromagnetic systems, it helps to first appreciate the role played by the Coulomb interaction and the symmetry principle in influencing a net magnetic moment in an excited helium atom. Writing out the possible choices for the total wavefunction for the two helium electron system as an outer product of the spatial (hydrogenic) and spinorial parts, with adherence to the symmetry principle, \(\Psi(r_1, r_2) = -\Psi(r_2, r_1)\), we have

\[
\begin{align*}
\Psi_{\text{para}}(r_1, r_2) &= \frac{1}{\sqrt{2}} [\psi_{100}(r_1)\psi_{nlm}(r_2) + \psi_{100}(r_2)\psi_{nlm}(r_1)] \otimes \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 - |\uparrow\rangle_2 |\downarrow\rangle_1], \\
\Psi_{\text{ortho}}(r_1, r_2) &= \frac{1}{\sqrt{2}} [\psi_{100}(r_1)\psi_{nlm}(r_2) - \psi_{100}(r_2)\psi_{nlm}(r_1)] \otimes |\uparrow\rangle_1 |\uparrow\rangle_2, \\
\Psi_{\text{ortho}}(r_1, r_2) &= \frac{1}{\sqrt{2}} [\psi_{100}(r_1)\psi_{nlm}(r_2) - \psi_{100}(r_2)\psi_{nlm}(r_1)] \otimes |\downarrow\rangle_1 |\downarrow\rangle_2, \\
\Psi_{\text{ortho}}(r_1, r_2) &= \frac{1}{\sqrt{2}} [\psi_{100}(r_1)\psi_{nlm}(r_2) - \psi_{100}(r_2)\psi_{nlm}(r_1)] \otimes \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 + |\uparrow\rangle_2 |\downarrow\rangle_1].
\end{align*}
\]
antisymmetric spatial states (so as to result in an overall antisymmetric wavefunction), have a lower energy than the parahelium states (1.1), described by the outer product of the antisymmetric spinorial singlet state and symmetric spatial states [Bandyopadhyay and Cahay, 2008],

\[
E_{\text{para}} = E_{100} + E_{nlm} + K_C + J_{\text{ex}},
\]

(1.3)

\[
E_{\text{ortho}} = E_{100} + E_{nlm} + K_C - J_{\text{ex}}.
\]

(1.4)

Here, \(E_{100}\) and \(E_{nlm}\) represent the hydrogenic (nuclear charge 2\(e\)) contribution to the helium energy, \(K_C\) accounts for the anticipated correction due to Coulomb repulsion,

\[
K_C = \int\int \frac{e^2 |\psi_{100}(r_1)|^2 |\psi_{nlm}(r_2)|^2}{|r_1 - r_2|} \, dr_1 dr_2,
\]

(1.5)

and \(J_{\text{ex}}\) is the exchange integral

\[
J_{\text{ex}} = \int\int \frac{e^2 \psi_{100}^*(r_1)\psi_{nlm}^*(r_1)\psi_{100}(r_2)\psi_{nlm}(r_2)}{|r_1 - r_2|} \, dr_1 dr_2.
\]

(1.6)

The energy difference between the parahelium and orthohelium states rests in the integral \(J_{\text{ex}}\), quantifying what is called the exchange interaction between spins, and reflects the Coulomb interaction energy between charge densities \(e\psi_{100}(r_1)\psi_{nlm}^*(r_1)\) and \(e\psi_{100}^*(r_2)\psi_{nlm}(r_2)\) (cf. Eq. (1.5)). For helium, \(J_{\text{ex}}\) is positive, and orthohelium states are energetically favored over parahelium states, wherefore the expectancy of a net magnetic moment is greater. Since the exchange energy term \(J_{\text{ex}}\) differentiating the parahelium states from the orthohelium states comes out only as a consequence of assembling the overall wavefunction for the helium system antisymmetrically ((1.1) and (1.2)) so as to adhere to the symmetry principle (or Pauli’s exclusion principle), it is apparent that the prevalence of a net magnetic moment in an excited helium atom \((J_{\text{ex}} > 0)\) is fundamentally a quantum effect. Though we focused exclusively on an excited helium atom, as the simplicity of the particular system lent way to a closed-form expression for \(J_{\text{ex}}\) and convenience in expounding the exchange interaction, we note that most isolated open-shell atoms exhibit a net magnetic moment in the ground state. The exchange interaction is the principal basis underlying Hund’s rule #1, that within each subshell electrons will singly occupy the orbitals to maximize the total spin, before doubly occupying the orbitals which reduces total angular momentum due to the pairing of necessarily opposite electron spins as underlined by Pauli’s exclusion principle. Subscribingly, heavy atoms with half-filled shells brandish the greatest magnetic moment. Molecules follow suit.
However, ferromagnetic materials are not isolated atoms or molecules, rather complexes of tightly bound atoms, molecules, or ions, where interactions are much further complicated by the extended structure. Most familiar ferromagnetic materials are metals with complex electronic band structures. Hybridization of electron orbitals typically prevents the development of spontaneous macroscopic magnetic moment that would occur on principles already outlined for the simple example of an excited helium atom. Nevertheless, for certain cases such as iron, nickel, cobalt, and many of their alloys, spontaneous magnetization persists despite band formation. The characteristic length scale quantifying the extent to which the exchange interaction manages to keep spins uniformly oriented within a ferromagnet is called the exchange length, and is typically on the order of 1–100 nm. While the magnetization $\mathbf{M}(\mathbf{r})$ within a homogeneous ferromagnetic body may cease to be uniform over distances greater than the exchange length, the magnetic moment density $M_s = \mathbf{M}(\mathbf{r})/|\mathbf{M}(\mathbf{r})|$ (saturation magnetization) necessarily remains constant for a fixed temperature.

In many cases, simplified models of ferromagnetism can be found useful. In the Stoner model, spin up and spin down electrons are regarded as free particles, and a vertical offset is introduced between the two bands to account for the exchange splitting responsible for the spontaneous spin imbalance (Fig. 1.2a). The Stoner model is the
The premise of derivations in section 2.1.8. The s-d model, on the other hand, assumes a strongly exchange-split localized d-band and a delocalized s-band, with weak coupling between the two (Fig. 1.2b). This model helps explain the spin-dependent scattering rates responsible for the giant magnetoresistance and tunneling magnetoresistance effects (section 12.1.1). More realistic descriptions of ferromagnetism can be obtained using the local spin density approximation (LSDA). The LSDA reveals that d-electrons in transition metals are in fact strongly interacting and itinerant, a point of once great contention [Moriya and Takahashi, 1984]. For many ferromagnetic systems first principles calculations can yield an accurate estimate of magnetic moment density, exchange length, susceptibility, and other relevant magnetic properties, including the Curie temperature $T_C$. Above this temperature, the spontaneous magnetic order is destroyed by thermal fluctuations and the ferromagnet transitions to paramagnetism with a susceptibility typically obeying the Curie-Weiss law, $\chi \propto (T - T_C)^{-1}$.

### 1.4 Antiferromagnetism

Antiferromagnetic materials usually do not exhibit net macroscopic magnetic moment, yet long range correlation between electron spins does exist. This is because in antiferromagnetic substances the spontaneous magnetic moment across one sublattice is typically counterbalanced by the oppositely oriented magnetic moment of another sublattice (Fig. 1.3a). In many antiferromagnets, oxygen anions situated intermittently between two magnetic sublattices mediate the spin-to-spin interaction (a phenomenon known as superexchange). Such substances are called antiferromagnetic oxides, and
include MnO, FeO, CoO, and NiO. Other examples are metallic antiferromagnets, FeMn, IrMn, and MnRh. The latter are commonly used to achieve exchange biasing important in magnetic recording heads and spin valve technology [Nogues and Schuller, 1999]. Above the Néel temperature $T_N$, antiferromagnets become paramagnetic with a susceptibility commonly following the Curie-Weiss relation, $\chi \propto (T - T_N)^{-1}$. A spin flop transition is also possible, whereby upon increasing the temperature the antiparallel magnetic moments acquire a common component along a preferred direction resulting in weak spontaneous magnetization (Fig. 1.3b).

1.5 Ferrimagnetism

Like antiferromagnets, ferrimagnetic materials are described as having two magnetic sublattices with macroscopically coherent and opposing spins. However, unlike in antiferromagnets, the magnitude of the magnetic moments on the respective sublattices differs, resulting in a net macroscopic magnetic moment (Fig. 1.4). Magnetite, long thought to be ferromagnetic, was the first identified ferrimagnet following Néel’s theory of ferrimagnetism and antiferromagnetism in the 1940s. Ferrimagnets are useful for a number of applications due to their high frequency response and low eddy current losses [O’Handley, 1999]. Ferrimagnetic materials have also been at the focus of much recent investigation into ultrafast magnetization switching where circularly polarized light is used to heat the structure to the angular momentum compensation point and pump in angular momentum to cause switching. The interplay between light and the different subsystems on different timescales in ferrimagnets such as GdFeCo is not yet well understood. Recently, non-polarized light (zero angular momentum) was demonstrated to deterministically induce picosecond switching in GdFeCo, provoking further speculation on the mechanisms involved in light-induced magnetization reversal [Ostler et al., 2012].
2 Micromagnetics: The Continuum Approach to Ferromagnetism

In the previous chapter we focused on interactions between magnetic moments on an atomic level and considered the electronic structure of ferromagnetic systems. While atomistic considerations and quantum mechanics provide deep insight into the workings of ferromagnetism, a more suitable framework was sought to account for magnetic phenomena on the mesoscale. Micromagnetics, as a discipline, originated from the need to explain domain wall formation, domain patterns, nucleation fields, reversal modes, and magnetization dynamics, in general. W. F. Brown laid down the foundations of micromagnetic theory through his formal treatment of interaction energies in which magnetic moment density and material parameters enter as continuous variables [Brown, 1978]. Equilibrium solutions for the magnetization configuration of a system can be found by solving Brown’s equations. Magnetization dynamics for a system out of equilibrium can be traced using the Landau-Lifshitz-Gilbert equation wherein the driving force is equal to the negative sum of the gradients of the different energy terms. The particular trajectory the magnetization takes, and the equilibrium state to which the magnetization ultimately relaxes, are determined by the competition between participating interactions. A practical introduction to the field of micromagnetics is therefore an overview of the various governing interactions.
2.1 Governing Interactions

Eleven interactions are presented. The first is the Zeeman interaction, being the simplest, followed by the magnetostatic interaction. Described next are the magnetocrystalline, magnetoelastic, and magnetoelastic interactions, as they all rely on spin-orbit coupling. The exchange interaction, the Ruderman-Kittel-Kasuya-Yosida interaction, and the interaction with spin currents are then covered. These three interactions are spin-transfer mediated, and are thus introduced in succession. Lastly, interactions with the heat bath, heat currents, and light are discussed.

All cited interactions can be incorporated, one way or another, into micromagnetics. Many of the interactions can be viewed in terms of the coupling between a magnetic moment and the interaction-specific magnetic field. The equation describing the torque on a magnetic moment $\mu$ due to an acting magnetic field $H$ is written as

$$\frac{d\mu}{dt} = -\gamma \mu \times H,$$

(2.1)

where $\gamma$ denotes the gyromagnetic ratio. If $H$ is the net (effective) magnetic field and is non-varying in time, the magnetic moment will precess about it at a fixed cone angle, as illustrated in Fig. 2.1a.

Dissipative processes involving the extraction of energy from the system cause the precession to damp out, which is seen as the spiraling-in of the magnetic moment onto the effective field (Fig. 2.1b). The governing equation of field-driven dynamics including
damping is the Landau-Lifshitz-Gilbert equation

\[
\frac{d\mu}{dt} = -\gamma \mu \times H + \alpha \frac{\mu}{|\mu|} \times \frac{d\mu}{dt},
\]  

(2.2)

where \( \alpha \) is the damping parameter. Equation (2.2) can explicitly be written as (see section 4.2)

\[
\frac{d\mu}{dt} = -\frac{\gamma}{1 + \alpha^2} \mu \times H - \frac{\alpha \gamma}{1 + \alpha^2} \frac{\mu}{|\mu|} \times \mu \times H.
\]  

(2.3)

As shown in section 2.2, all interactions described by an energy functional taking the magnetic moment density as input can be regarded as influencing a magnetic moment through an associated magnetic field according to (2.3).

Note that the damping torque term preserves the length of the magnetization vector, and hence ensures a constant saturation magnetization per given temperature. Note also that it does not preserve time reversal symmetry, as expected in descriptions of dissipative processes. For a discussion of the possible forms of damping terms, see [Berkov, 2007], and references therein. Dissipation considerations are revisited in section 2.1.9 and chapter 5. The preservation of magnetization magnitude as guaranteed by (2.2) and (2.3) is respectful of the exchange interaction (section 1.3, section 2.1.6), which calls for atomic spins to point cooperatively within regions of sub-exchange length dimensions. The orderliness of atomic spins determines the magnetic moment density, and hence \(|\mu|\) of a uniformly magnetized region. Changing the temperature affects the level of order in the spin system and consequently the moment density and \(|\mu|\). The dynamical equation which includes the effect of temperature on \(|\mu|\) is presented in chapter 5. For now, it will be sufficient to consider (2.3), and realize that the configuration in which \(\mu\) is oriented along the effective field \(H\) corresponds to a micromagnetic energy minimum.

Lastly, we refer to Fig. 2.1c, noting that a magnetic field cannot be affiliated with certain interactions, in which case their effect on the dynamics of magnetic moments enters the governing equation as an additive torque term,

\[
\frac{d\mu}{dt} = -\frac{\gamma}{1 + \alpha^2} \mu \times H - \frac{\alpha \gamma}{1 + \alpha^2} \frac{\mu}{|\mu|} \times \mu \times H + \tau.
\]  

(2.4)

In (2.4), \(H\) is the effective magnetic field, i.e., the net acting field coming from the various interactions, and \(\tau\) is the net torque produced by interactions whose contribution cannot be expressed in terms of field.
Figure 2.2: Two magnetic moments interacting through their stray magnetic fields.

2.1.1 Zeeman Interaction

The Zeeman interaction is the interaction between an applied field \( H_a \) (Oe) and a magnetic moment \( \mu \) (emu). The applied field \( H_a \) is sometimes also referred to as the Zeeman field. For a magnetic dipole moment \( \mu \) under a field \( H_a \) the interaction energy is expressed as

\[
E = -\mu \cdot H_a,
\]

while for an extended magnetic moment density, represented by the magnetization vector \( M \) (emu/cm\(^3\)), the energy is

\[
E = -\int_V M(\mathbf{r}) \cdot H_a(\mathbf{r}) \, d^3r.
\]

As indicated by the equations, the energy is lowest when the magnetic moment is oriented with the field, and maximum when \( \mu \) (or \( M \)) is oriented opposite to \( H_a \). While the Zeeman interaction usually involves an external field, such as can be applied over a sample using an electromagnet or field lines, the energy expression in (2.6) can also be used to include contributions from self-generating fields due to eddy currents or applied currents flowing through the magnet.

2.1.2 Magnetostatic Interaction

A magnetic moment produces a magnetic field. Two magnetic moments, \( \mu_1 \) and \( \mu_2 \) (Fig. 2.2), interact through the magnetic fields they produce, \( H_1 \) and \( H_2 \). The total
magnetostatic energy for two magnetic dipole moments can be expressed, analogous to (2.5), as

$$E_{ms} = -\mu_1 \cdot H_2(r_1),$$  \hspace{1cm} (2.7)

or, equivalently,

$$E_{ms} = -\mu_2 \cdot H_1(r_2),$$  \hspace{1cm} (2.8)

where $H_2(r_1)$ is the field on $\mu_1$ as generated by $\mu_2$, and $H_1(r_2)$ is the field on $\mu_2$ due to $\mu_1$. The equivalence between equations (2.7) and (2.8) is known as the reciprocity theorem of magnetostatics. The total energy can be alternatively expressed as

$$E_{ms} = -\frac{1}{2} \left[ \mu_1 \cdot H_2(r_1) + \mu_2 \cdot H_1(r_2) \right].$$  \hspace{1cm} (2.9)

For the case of multiple dipole moments, this generalizes to

$$E_{ms} = -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1 \atop j \neq i}^{N} \mu_i \cdot H_j(r_i),$$  \hspace{1cm} (2.10)

where the self-interaction for point-dipoles is excluded. For an extended moment density (magnetization) $M$, the magnetostatic energy takes the form

$$E_{ms} = -\frac{1}{2} \int_V M(r) \cdot H_{ms}(r) \, d^3r.$$

Here, $H_{ms}(r)$ is the demagnetization field at coordinate $r$ due to the magnetization throughout volume $V$,
The effective magnetic volume and surface charge densities are defined as

\[ \rho_M = -\nabla \cdot \mathbf{M}, \]  

(2.13)

\[ \sigma_M = \hat{n} \cdot \mathbf{M}, \]  

(2.14)

where \( \hat{n} \) is the outward unit normal to the surface \( S \) bounding volume \( V \) containing magnetization \( \mathbf{M} \). The magnetic-flux density is obtained from \( \mathbf{B} = \mathbf{H} + 4\pi \mathbf{M} \). Since \( \mathbf{M} \times \mathbf{B} = \mathbf{M} \times \mathbf{H} \), distinguishing between the \( \mathbf{H} \)- and \( \mathbf{B} \)-field will only be important in select cases (see section 5.3).

We now turn to some examples to gain an intuitive understanding of the effect the magnetostatic interaction has on the magnetization configuration of various samples. First, consider a uniform array of magnetic nanoislands, as illustrated in Fig. 2.3a. Assume sub-exchange length dimensions so that each island is strictly single domain and can be regarded as a magnetic dipole moment. The magnetostatic energy in this case is minimized when adjacent nanoislands have opposite moment directions since such a configuration maximizes flux closure (Fig. 2.3a). For this reason, the magnetostatic interaction is said to result in antiferromagnetic coupling between moments (the antiparallel configuration
being analogous to the microscopic order of antiferromagnets; see Fig. 1.3). If the discreteness of the system of nanoislands in Fig. 2.3a is abolished by interconnecting the islands so as to form a continuous nanowire (NW), the exchange interaction will prevent the antiparallel configuration from remaining the most energetically favorable, as this would result in multiple domain walls over a short-range with a high associated energy cost. The minimum energy state for the NW is achieved when the magnetic moment points along the long axis of the wire (Fig. 2.3b).

Generally, the magnetostatic interaction promotes alignment of the magnetization with the axial direction of the magnetic sample, as this minimizes effective magnetic surface charges \( \sigma_M \); see (2.14). A great example is a torus or ring structure (Fig. 2.4a) where the magnetization may close in on itself (assuming dimensions sufficiently greater than the exchange length) to yield virtually no effective surface charges, \( \sigma_M \). For the so called onion state, involving two domain walls (Fig. 2.4b), the magnetization is also predominantly along the axial direction of the ring, with a noticeable deviation occurring only at the location of the walls, where \( \sigma_M \) is non-vanishing. A similar example to that in Fig. 2.4a is a magnetically soft nanodisk with a diameter in extent of several exchange lengths. The magnetization in this case, too, tends to close in on itself; however, this implicates a magnetic vortex at the disk’s center, with large \( \sigma_M \) (Fig. 2.5).

These examples illustrate why the magnetostatic interaction is said to bestow onto a magnetic system shape anisotropy. In many cases, such as films and nanowires, shape anisotropy acts similar to magnetocrystalline anisotropy (section 2.1.3), and the two terms

**Figure 2.5:** Magnetic nanodisk in a vortex state. The competition between the magnetostatic interaction and the exchange interaction (section 2.1.6) determines the diameter of the vortex core.
Figure 2.6: Two stable magnetization configurations for a plate with perpendicular uniaxial magnetocrystalline anisotropy.

may be merged into a single effective anisotropy contribution for back-of-the-envelope calculations.

2.1.3 Magnetocrystalline Interaction

The spin-orbit (SO) interaction is the relativistic interaction between an electron spin and a potential, which, in the reference frame of the orbiting electron, is seen as an effective magnetic field. When the potential originates from the crystal lattice, the SO interaction may more specifically be called the magnetocrystalline interaction. In this case, the interaction symmetry reflects the symmetry of the crystal structure. Most important for magnetic recording applications are magnetic structures characterized by high uniaxial symmetry. Such structures are said to possess strong uniaxial magnetocrystalline anisotropy, meaning that there is a well-defined direction with respect to the crystal along which the magnetic moments (spins) prefer to point (Fig. 2.6). The axis defining the preferential direction of magnetic moments is called the easy axis. The magnetocrystalline anisotropy energy is minimized when the moments point along the easy axis. The energy for a single moment \( \mathbf{\mu} \) is given as

\[
E_{\text{anis}} = -KV \left( \hat{\mathbf{\mu}} \cdot \hat{\mathbf{k}} \right)^2 = -KV \cos^2 \theta, \tag{2.15}
\]

where \( K \text{ (erg/cm}^3) \) is the magnetocrystalline anisotropy energy density, \( V \) is the volume occupied by moment \( \mathbf{\mu}, \hat{\mathbf{\mu}} = \mathbf{\mu}/|\mathbf{\mu}|, \hat{\mathbf{k}} \) is the easy axis direction, and \( \cos \theta = \hat{\mathbf{\mu}} \cdot \hat{\mathbf{k}}. \)
Figure 2.7: Competition between the Zeeman and magnetocrystalline interactions. The energy barrier $\Delta E$ separating two stable states (see Fig. 2.6) is zero when the applied field amplitude reaches the threshold for magnetization reversal.

Assuming $\hat{k} = \hat{z}$, the energy is minimum for two possible orientations of $\hat{\mu}$, namely $\hat{\mu} = \hat{z}$ and $\hat{\mu} = -\hat{z}$. Both configurations are stable, whence we say uniaxial magnetic systems render bistability to the magnetization (Fig. 2.6). This bistability is exploited in magnetic recording, where upward and downward magnetized particles encode bits 0 and 1 (binary information storage). When a new sequence of bits is to be written, an applied field (supplied by the recording head; section 9.1.3) is used to orient the magnetic moments in the needed direction. When reorienting a moment, it is important that the applied field is sufficiently large, else magnetocrystalline anisotropy will dominate over the Zeeman interaction (section 2.1.1) and prevent switching. The competition between the Zeeman interaction and the magnetocrystalline interaction is illustrated in Fig. 2.7, which shows the Zeeman energy, magnetocrystalline anisotropy energy, and the net energy as a function of $\theta$ for a single magnetic moment under applied fields of varying strengths.

The uniaxial anisotropy energy for the more general case of an extended moment density $\mathbf{M}(\mathbf{r})$ is given by

$$ E_{\text{anis}} = -\int_V K(\hat{\mathbf{m}} \cdot \hat{k})^2 dV, \quad (2.16) $$

where $\hat{\mathbf{m}} = \mathbf{M}/|\mathbf{M}| = \mathbf{\mu}/|\mathbf{\mu}| = \hat{\mu}$. In some materials, $K < 0$, and a magnetization...
perpendicular to the uniaxial direction, $\hat{k}$, is favored. Ferromagnets of this kind are called easy-plane-type ferromagnets, to distinguish them from easy-axis-type ferromagnets, for which $K > 0$. When $K < 0$, $\hat{k}$ represents the hard-axis direction, and higher order terms must often be included in the energy expression, as their contributions may no longer be insignificant.

Cubic anisotropy and higher order terms can easily be put to expression by considering time reversal symmetry [Landau and Lifshitz, 1984]

$$T^{-1}: \quad J \rightarrow -J, \quad M \rightarrow -M, \quad H \rightarrow -H, \quad E \rightarrow E.$$  \hspace{1cm} (2.17)

Here, $J$ stands for the electric currents in a system, $H$ represents the magnetic fields, $M$ is the magnetization, and $E$ is the energy. Upon time reversal, the flow of charge carriers reverses, giving $T^{-1}: J \rightarrow -J$. Since a magnetic moment is due to orbital or intrinsic angular momentum, we have as a consequence $T^{-1}: M \rightarrow -M$. Similarly, $T^{-1}: H \rightarrow -H$, due to the fact that magnetic fields originate from currents and the magnetization. The energy, on the other hand, is invariant to time reversal, as attested by the fact that the direction of time cannot be determined based on the observation of a system in equilibrium. The possible forms of magnetocrystalline anisotropy energy obeying $T^{-1}$ can be concisely written, using Einstein summation convention, as

$$E_{\text{anis}} = K^{(pqr)}_{ijk} m_i^p m_j^q m_k^r \mid p + q + r = 2k, \quad k \in N_1,$$  \hspace{1cm} (2.18)

where $i, j$ and $k$ represent the three spatial components, commonly denoted as $x, y$ and $z$, while $p, q$ and $r$ are integers whose sum is a positive even number. This condition ensures that the energy remains invariant (no change in sign) under $T^{-1}$. When modeling magnetic materials, it is important to consider the crystal symmetry, which puts additional constraints on the form of the above expression [Landau and Lifshitz, 1984]. All crystals obey uniaxial symmetry. For tetragonal crystals, the higher order invariants are $(m_x^2 + m_y^2)^2$ and $m_x^2 m_y^2$, for hexagonal crystals $(m_x^2 + m_y^2)^2$ and $(m_x + im_y)^6 + (m_x - im_y)^6$, and for rhombohedral crystals $(m_x^2 + m_y^2)^2$ and $m_z[(m_x + im_y)^3 + (m_x - im_y)^3]$. At surfaces and interfaces, the form of the magnetocrystalline anisotropy energy reflects the reduced or broken symmetry [O’Handley, 1999].

### 2.1.4 Magnetoelastic Interaction

In the previous section we introduced the notion of the spin orbit (SO) interaction, but focused immediately thereafter on magnetocrystalline anisotropy. In this section, we
describe the magnetoelastic interaction, which is tied to the SO interaction and related to
the magnetocrystalline interaction. Several phenomena are ascribed to the magnetoelastic
interaction. The most familiar is magnetostriction, as first observed by Joule (1842),
which manifests as a magnetic field-induced strain. Positive Joule magnetostriction
implies that a material expands in the direction of the applied field, whereas negative
Joule magnetostriction implies contraction in the field direction (Fig. 2.8). In either event,
the total volume is preserved, meaning that Joule magnetostriction implicates isochoric
deformation. The inverse phenomenon, namely, the change in the magnetization due to
an applied stress, is called the Villari effect (1865). Both phenomena are characterized
by quadratic coupling between the magnetization and strain, which is why the arrows
in Fig. 2.8 are double-headed – to indicate that the orientation (sign) of the applied
field bears no significance. This is to be contrasted with piezomagnetism, a linear effect,
where a change in field orientation produces strain of the opposite sense. The utility of
Joule magnetostriction and the Villari effect, and magnetoelastic effects in general, is
evidenced by the number of technological applications in service today – transformers,
actuators, and sensors representing familiar examples.

The occurrence of magnetoelastic effects can in part be apprehended intuitively
by recognizing the intimate dependence of magnetism on crystal structure and lattice
parameters and by observing that strain implies structural deformation and a change
in potential that can affect magnetic properties through orbital reconfiguration and SO

Figure 2.8: (a) Positive Joule magnetostriction: elongation in the direction of the
applied magnetic field. (b) Negative Joule magnetostriction: contraction in the direction
of the applied magnetic field.
coupling. Magnetoelastic effects in extended systems can be further complicated by
the magnetic domain structure, whose response to magnetic fields and stress can be
convoluted. The $\Delta E$ magnetoelastic effect, and its conjugate, which couple magneto-
crystalline anisotropy and elasticity, can add to the behavioral complexity and involution
in materials where these effects are dearly experienced, such as iron. Other magneto-
elastic phenomena include volume magnetostriction (where field-induced deformation is
isotropic and anisochoric), its inverse, the Nagaoka-Honda effect, and the Wiedemann
effect, describing the twisting induced by a helical magnetic field/anisotropy, as well as
its inverse, the Matteuci effect.

Magnetoelasticity is exceptionally prominent in rare-earth magnets, which often
serve as model systems for studying phenomena modulated by magnetoelastic effects,
such as magnon-phonon interactions. Rare-earth magnets are widely used in industry
today. Terfenol-D ($\text{Tb}_x\text{Dy}_{x-1}\text{Fe}_2$) is a familiar rare-earth alloy featuring an exquisitely
high magnetostriction coefficient of $\lambda = \Delta l/l \approx 2000 \times 10^{-6}$.

Magnetoelastic effects are also important in magnetic memory and processing
applications where devices sport nanoscale dimensions. For instance, fabrication of
nanowires via patterning causes symmetry breaking at exposed edges which results in
strain relaxation that can affect magnetic properties, including the magnetic anisotropy
direction [Arnaudas et al., 2011]. Structural defects in nanowires can also be sources of
stress that can couple to the magnetization response via the magnetoelastic interaction
and cause domain wall pinning. In multilayer heterostructures, interfacial stress can affect
magnetization equilibrium states and dynamics. While the magnetoelastic contribution
here can be seen as detrimental for device performance, it can also be favorably exploited
to achieve desirable device behavior.

2.1.5 Magnetoelastic Interaction

The magnetoelastic interaction is manifest whenever the magnetic and electric
order parameters are coupled. Such coupling may be direct, as in single-phase materials
boracite ($\text{Ni}_3\text{B}_7\text{O}_{13}\text{I}$) and bismuth ferrite ($\text{BiFeO}_3$), or strain-mediated, as in ferromag-
netic/ferroelectric heterostructures such as $\text{CoPd/PZT}$ ($\text{PZT} = \text{Pb}[\text{Zr}_x\text{Ti}_{1-x}]\text{O}_3$) [Eeren-
stein et al., 2006]. Systems of the latter category are called synthetic multiferroics, and
can exhibit significantly greater ordering temperatures and magnetoelastic effects than
currently known single-phase systems. For this reason, we limit our discussion to the
strain-mediated magnetoelectric interaction.

Consider an epitaxially grown ferromagnetic/ferroelectric bilayer, as illustrated in Fig. 2.9. We shall assume that the ferroelectric material exhibits sufficient piezoelectricity, so that the application of a voltage on this layer induces an appreciable strain. Owing to the coupling interface between the ferroelectric and ferromagnetic layers, the strain field extends throughout the bilayer. If the magnetoelastic interaction (section 2.1.4) in the ferromagnet is strong, the magnetization can be influenced or even switched. Conversely, the application of a magnetic field on the multiferroic bilayer induces a strain in the ferromagnet which spreads across the mutual interface to the ferroelectric layer and can affect its electric polarization. Both phenomena are attractive for magnetic memory and logic applications, since a multiferroic cell could allow for both electrical transcription and electrical control of magnetization states (for examples of magnetic logic implementations using multiferroic cells, see [Khitun et al., 2008, Khitun and Wang, 2011]). Other applications include high-grade multiferroic field sensors as a cheaper alternative to superconductor quantum interface devices (SQUIDs), and optical devices in which the interaction between the magnetization and the optical field (section 2.1.11) is modulated via the magnetoelectric effect [Eerenstein et al., 2006].

2.1.6 Exchange Interaction

In strongly magnetic systems, the exchange interaction is responsible for maintaining macroscopic magnetic order, and is the source of ferromagnetism, antiferromagnetism, and ferrimagnetism. The origins of the exchange interaction have been discussed in section 1.3. A description of the exchange energy between adjacent spins on the crystal
lattice is given by the atomistic Heisenberg Hamiltonian

\[ H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j, \]  

(2.19)

where \( J_{ij} \) is the coupling energy (exchange integral) between atomic spins \( \mathbf{s}_i \) and \( \mathbf{s}_j \).

Since the exchange integral quantifies the spatial overlap of the wavefunctions between spins (section 1.3), \( J_{ij} \) for many lattice systems can be assumed zero when \( i \) and \( j \) correspond to non-nearest neighbor lattice sites. Interatomic exchange coupling in such cases can be illustrated by a lattice of spins whose rotational degrees of freedom are coupled through effective springs (Fig. 2.10). The springs prevent large deviations in spin direction from one lattice site to the next, thus guaranteeing local magnetization uniformity. However, small correlated deviations can lead to magnetization nonuniformity on a larger scale. A basic example is a domain wall (DW) in a magnetic strip with perpendicular magnetocrystalline anisotropy, as shown in Fig. 2.11.

To account for the DW, it is more convenient to express the exchange interaction in continuum form, which can be derived from the atomistic Heisenberg Hamiltonian [d’Aquino, 2004]. For the case of an isotropic medium, the micromagnetic exchange interaction takes the form

\[ E_{\text{ex}} = \int_V A (\nabla \mathbf{m})^2 \, dV. \]  

(2.20)
Here, $\hat{m}$ is the unit magnetization direction, $(\nabla \hat{m})^2 = |\nabla m_x|^2 + |\nabla m_y|^2 + |\nabla m_z|^2$, and $A$ is the exchange constant or energy density (related to $J$; see [d’Aquino, 2004]).

The DW in Fig. 2.11 can be shown to result from the competition between the exchange and magnetocrystalline interactions, when one end of the strip is magnetized up and the other end down. Since the exchange interaction opposes large gradients in magnetization direction, it tends to dilate DWs. In contrast, the magnetocrystalline interaction promotes sharp transitions from one domain to the next in order to minimize the quantity of moment that is at an angle with respect to the easy axis. The compromise between the two interactions defines the DW length

$$l_{DW} \approx \pi \sqrt{\frac{A}{K}},$$

(2.21)

and the DW surface energy density

$$\sigma_{DW} \approx 4\sqrt{AK},$$

(2.22)

where $K$ (erg/cm$^3$) is the magnetocrystalline energy density [O’Handley, 1999].

The competition between the exchange interaction and the magnetostatic, magnetocrystalline, and Zeeman interactions, allows for diverse magnetization dynamics and far more exotic equilibrium configurations than shown in the example of Fig. 2.11. Figure 2.12 shows the playful (albeit static) magnetization pattern that develops in a $0.2\mu m \times 0.2\mu m \times 8\mu m$ nanowire with tilted uniaxial magnetocrystalline anisotropy. Even more interesting is a metastable configuration in a nanowire of same dimensions, but featuring cubic anisotropy (Fig. 2.13a). For this case, spin configurations of cross-sections
Figure 2.12: Domain pattern in a magnetic nanowire with tilted easy axis illustrating the competition between the magnetocrystalline, magnetostatic, and exchange interactions.
Figure 2.13: Domain structure in a single crystal nickel nanowire illustrating the competition between the (a) magnetocrystalline, magnetostatic, exchange, and (b) Zeeman interactions.
sampled along the nanowire axis reveal a periodic change in the vortex chirality (right/left handedness) occurring every $\sim 200$ nm. Figure 2.13b shows the equilibrium magnetization configuration under an applied field of 1 kOe. More information can be found in [Chan et al., 2012, Kan et al., 2013].

### 2.1.7 RKKY Interaction

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction represents the interaction between localized inner-shell electron spins mediated by conduction electron spins. The interaction is important because it allows magnetic layers to be indirectly exchange coupled through a thin ($\sim 1$ nm) intervening nonmagnetic spacer layer (Fig. 2.14a). Since the conduction electrons are responsible for mediating the interaction across the spacer, the strength of coupling may be tuned through spacer layer thickness and composition. For these reasons, RKKY coupling is often referred to as indirect, modulated, or interlayer exchange coupling. It has been shown for many systems that the strength of RKKY coupling oscillates smoothly and that the sense of coupling changes as the spacer layer thickness is modulated (Fig. 2.14b) [Parkin et al., 1990, Bruno and Chappert, 1992]. This means that magnetic layers can be coupled either ferromagnetically or antiferromagnetically across the spacer layer (to promote parallel or antiparallel alignment of magnetization). This was finely illustrated in an experiment where two layers of Fe were separated by a wedge-shaped Cr spacer layer to result in periodic ferromagnetic/antiferromagnetic (FC/AFC) coupling (Fig. 2.14c) [Unguris et al., 1991].

The interlayer exchange interaction energy for two magnetic layers separated by a nonmagnetic spacer layer is micromagnetically expressed as

$$E_{\text{RKKY}} = -\int_S J \hat{\mathbf{m}}_1 \cdot \hat{\mathbf{m}}_2 \, dS,$$

where $J$ (erg/cm$^2$) is the coupling strength (energy density), $\hat{\mathbf{m}}_1(r) = M_1(r)/|M_1(r)|$ and $\hat{\mathbf{m}}_2(r) = M_2(r)/|M_2(r)|$ represent the interfacial magnetization directions of the two magnetic layers, respectively, and $S$ denotes the coupling surface and domain of integration. When $J > 0$, the interlayer coupling is ferromagnetic, promoting parallel magnetization alignment across the interface. For $J < 0$, the coupling is antiferromagnetic, and an antiparallel configuration is favored.

When many oscillations or fluctuations of the sign of coupling occur over distances smaller than the exchange length (e.g., due to interface roughness), frustration (the
Figure 2.14: (a) Two ferromagnetic layers indirectly exchange coupled across a nonmagnetic spacer layer. (b) Example of the dependence of the coupling parameter (energy density) on spacer layer thickness. (c) Periodic ferromagnetic/antiferromagnetic coupling between two magnetic layers exchange coupled across a wedge-shaped spacer [Unguris et al., 1991].

inability to minimize both the bulk (intralayer) exchange and interlayer exchange energies) results in biquadratic coupling which promotes perpendicular alignment between the two magnetic layers [Moser et al., 2003]. The energy for biquadratic coupling is given by

$$E_{\text{bq}} = \int_S J_{\text{bq}} (\hat{\mathbf{m}}_1 \cdot \hat{\mathbf{m}}_2)^2 dS,$$

(2.24)

where $J_{\text{bq}}$ (erg/cm$^2$) quantifies the biquadratic coupling strength.

The competition between indirect interlayer exchange and the interactions discussed in the preceding sections adds to the variety of possible magnetization patterns in magnetic systems, as well as to the richness of possible dynamical responses. In Co/Pt or Co/Pd multilayer islands, for example, modulating the spacer thickness allows one to tune the ratio of vertical to lateral exchange in order to achieve different reversal modes (Fig. 2.15a) [Tudosa et al., 2012]. In an indirectly coupled hard/soft bilayer, and optimum interlayer exchange coupling strengths exists which minimizes the threshold
Figure 2.15: (a) Reversal modes in Co/Pd multilayer islands depend on the relative strength of (bulk) lateral and (indirect) vertical exchange. (b) In an indirectly coupled hard/soft composite, interlayer exchange coupling strength can be optimized to minimize the switching field. (c) Compensation of dipolar coupling through lateral and vertical exchange interactions in an array of nanoislands indirectly coupled to a continuous magnetic layer helps narrow the switching field distribution.
field required for magnetization switching (Fig. 2.15b) without affecting thermal stability [Suess, 2007]. An array of magnetic nanoislands indirectly coupled to a continuous capping layer (Fig. 2.15c) provides a means toward narrow switching field distributions owing to the compensation of dipolar coupling through lateral and vertical exchange interactions [Li et al., 2009a]. The delicate interplay between interlayer exchange and magnetostatic interactions is neatly displayed in the domain wall structure undergoing a phase-transitions as the layer thickness is varied in the AF coupled multilayers studied in [Hellwig et al., 2003].

2.1.8 Interaction with Spin Currents

In describing the RKKY interaction (section 2.1.7), it was noted that indirect interlayer exchange coupling is mediated by conduction electrons across the spacer layer. In bulk (intralayer) exchange, local magnetization misalignments generate internal spin currents which tend to restore magnetization uniformity [Stiles and Miltat, 2006]. Spin currents are therefore at the root of exchange interactions. This section describes specifically the interaction between externally injected spin currents and the magnetization.

Consider first a single uniformly oriented ferromagnet situated between the two nonmagnetic metallic leads (Fig. 2.16). When a voltage is applied across the device, an electric current develops. Since in normal metals (NMs), spin up and spin down states have an equal probability of being occupied, the electric current in the leads in Fig. 2.16 (sufficiently far away from the ferromagnet) has a zero spin polarization. However, in the ferromagnet (FM), the degeneracy between spin up and spin down states is lifted due to the strong exchange interaction (section 1.3), and this spin imbalance results in a spin polarized current within the ferromagnet. Within the Stoner model (Fig. 1.2a), the spin...
current is explained as a consequence of the population imbalance of spin up and spin down free electrons (here also called majority and minority carriers). From the perspective of the s-d model (Fig. 1.2b), the imbalance between majority and minority carriers (spin up and spin down itinerant s-band electrons) is insignificant, but the exchange splitting in the localized d-band is strong, resulting in a greater density of minority d-band states at the Fermi level to which s-band electrons can scatter. Since the frequency of scattering from the conducting s-band to the localized d-band depends on the density of available states in the d-band (Fig. 1.2b), the majority carriers will be less likely to scatter, and their flow will be less impeded by scattering than that of the minority carriers, again implying spin polarization of current within the ferromagnet.

As the electrons exit the ferromagnet and enter the right metallic lead, the spin polarization of the current will persist if the FM/NM interface does not introduce overmuch spin-flip scattering. Once the spin current is injected into the normal metal, its polarization falls off with increasing distance from the ferromagnet, as scattering works to balance the spin populations in the absence of exchange splitting. The polarization profile in the metallic lead can be estimated from the electron drift velocity and the spin-flip time [Zutic et al., 2004, Fabian et al., 2007].

A spin current also exists in the left metallic lead near the interface through which electrons enter the ferromagnet. The spin current here results from the conductance mismatch in spin up and spin down bands between the normal metal and ferromagnet. As a consequence of the mismatch, spin down (minority) electrons are more likely to reflect off the interface due to the inability to assume an unoccupied state in the ferromagnet. Such reflection results in spin accumulation at the NM/FM interface, the polarization of which tapers off down the lead away from the ferromagnet. The extent of this polarization profile is characterized by the spin diffusion length [Zutic et al., 2004, Fabian et al., 2007].

The ability of an unpolarized current of electrons to attain spin polarization on passing through a ferromagnet implies that angular momentum can be transferred between the incident electrons and the ferromagnetic lattice. By conservation of angular momentum, this means that the lattice must be capable of absorbing the angular momentum from the itinerant electrons. This is known as the spin transfer torque (STT) effect. It has great technological implications (sections 12.1.2, 12.1.3, 12.1.4, 13.1.1, 13.1.2) since it offers a means to use currents to locally manipulate magnetization states of magnets, as originally exemplified by [Berger, 1996, Slonczewski, 1996] in the following
Consider a NM/FM1/NM/FM2/NM junction (Fig. 2.17) through which current is passed, and assume the flow of electrons to be from left to right. Both ferromagnets FM1 and FM2 are considered soft and uniformly magnetized with a vertical easy axis established by shape anisotropy. The first thicker ferromagnet FM1 serves only to polarize the current, as it is too big and its moment too great to be noticeably affected by the transfer of angular momentum from the itinerant electrons. The second much thinner ferromagnet FM2, onto which the spin polarized current is incident from FM1, has a far lower magnetic moment which can be influenced by the STT effect. The STT effect can be used to switch FM2, provided that the angular momentum supplied to the magnet by the polarized current is pumped in at a rate that surpasses dissipation, and that the current is spin-polarized in the proper direction (section 12.1.2). An alternative application of spin transfer torque in the present geometry is to drive FM2 into steady-state precession (see section 12.1.4), which is achieved when the rate of angular momentum pumped into the magnet equals the rate of angular momentum dissipation due to damping. When both FM1 and FM2 are thin, simultaneous precession of the magnetization of both layers is possible, a dynamic known as pin-wheel motion [Slonczewski, 1996, Urazhdin et al., 2009].

A simple one-dimensional toy model originally employed [Berger, 1996, Slonczewski, 1996, Ralph and Stiles, 2008] to demonstrate quantum mechanically the transfer of angular momentum between a ferromagnet and itinerant spins goes as follows. Consider the spin dependent potential illustrated in Fig. 2.18a, modeling a NM/FM/NM junction with an upward oriented (in terms of angular momentum) ferromagnet. Both the spin up and spin down potentials are zero within the metal, while the spin down potential is

---

**Figure 2.17:** Spin valve: a ferromagnetic/normal metal/ferromagnetic junction connected to nonmagnetic leads.
Figure 2.18: (a) Spin-dependent potential (left); incoming electron current with spin direction indicated by red arrow (right). (b) Electron current, its spin up and down components, and the $z$-component of the spin current at incidence, transmission, and reflection. (c) The incident, within-the-barrier, and transmitted spin current. (d) The incident and reflected spin current. (e) Spin torque within the region $-w/2 < x < -w/2 + \lambda$ as a function of $\lambda$. 
stepped up in the region occupied by the ferromagnet to reflect exchange splitting therein. Assuming spins incident from the left with wave vector $k$, we have

$$\psi_{\text{in}} = \frac{1}{\sqrt{\Omega}} e^{ikx} \begin{pmatrix} a \\ b \end{pmatrix},$$

(2.25)

where $\begin{pmatrix} a \\ b \end{pmatrix}$ is the spinorial part of the two component spinor wavefunction given in the $z$-basis, and $\sqrt{\Omega}$ is the normalization. The discussion can be simplified to incident electrons with spin direction confined to the $xz$ plane, so that $\begin{pmatrix} a \\ b \end{pmatrix} \rightarrow \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}$, where polar angle $\theta$ defines the direction of incident spins. The incident and reflected wavefunctions in the left metal lead, the wavefunction within the ferromagnet, and the transmitted wavefunction in the right metal lead, are

$$\psi_{\text{in}} = \frac{1}{\sqrt{\Omega}} e^{ikx} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix},$$

(2.26)

$$\psi_{\text{rej}} = \frac{1}{\sqrt{\Omega}} e^{-ikx} \begin{pmatrix} R_\uparrow \\ R_\downarrow \end{pmatrix},$$

(2.27)

$$\psi_{\text{barr}} = \frac{1}{\sqrt{\Omega}} \left( \begin{pmatrix} A_\uparrow e^{ik_\uparrow x} \\ A_\downarrow e^{ik_\downarrow x} \end{pmatrix} + \frac{1}{\sqrt{\Omega}} \begin{pmatrix} B_\uparrow e^{-ik_\uparrow x} \\ B_\downarrow e^{-ik_\downarrow x} \end{pmatrix} \right),$$

(2.28)

$$\psi_{\text{trans}} = \frac{1}{\sqrt{\Omega}} e^{ikx} \begin{pmatrix} T_\uparrow \\ T_\downarrow \end{pmatrix}.$$  

(2.29)

Though we plotted in Fig. 2.18a a spin-dependent potential with zero barrier height for the spin-up electrons ($V_\uparrow = 0$), and a positive barrier for the spin-down electrons ($V_\downarrow > 0$), equations (2.26)–(2.29) remain valid for arbitrary $V_\uparrow$ and $V_\downarrow$. In the case the barrier height of a spin species is greater than the kinetic energy on incidence ($V_{\uparrow(\downarrow)} > \frac{k_{\uparrow(\downarrow)}^2 \hbar^2}{2m}$, where $m$ is the electron mass, and $\hbar$ is the reduced Planck’s constant), we may conveniently substitute $ik_{\uparrow(\downarrow)} \rightarrow -k_{\uparrow(\downarrow)}$. The same amplitude of wavevector $k$ used for incident, reflected, and transmitted wavefunctions in Eqs. (2.26), (2.27), and (2.29) reflects the assumption of elastic scattering. The total wavefunction is

$$\psi = \begin{cases} 
\psi_{\text{in}} + \psi_{\text{rej}}, & x \leq -w/2, \\
\psi_{\text{barr}}, & -w/2 < x < w/2, \\
\psi_{\text{trans}}, & x \geq w/2,
\end{cases}$$

(2.30)
where \( w \) denotes the thickness of the ferromagnet. Coefficients \( R\uparrow(\downarrow), A\uparrow(\downarrow), B\uparrow(\downarrow) \) and \( T\uparrow(\downarrow) \) are obtained from the consideration of the continuity of the wavefunction,

\[
\psi_{\text{in}} + \psi_{\text{refl}} |_{x = -\frac{w}{2}} = \psi_{\text{barr}} |_{x = -\frac{w}{2}},
\]

\[
\psi_{\text{barr}} |_{x = \frac{w}{2}} = \psi_{\text{trans}} |_{x = \frac{w}{2}},
\]

and its derivative with respect to \( x \),

\[
\psi^{'}_{\text{in}} + \psi^{'}_{\text{refl}} |_{x = -\frac{w}{2}} = \psi^{'}_{\text{barr}} |_{x = -\frac{w}{2}},
\]

\[
\psi^{'}_{\text{barr}} |_{x = \frac{w}{2}} = \psi^{'}_{\text{trans}} |_{x = \frac{w}{2}}.
\]

With the coefficients solved for, the wavefunction is entirely known, and the spin current can be calculated as

\[
Q = \text{Im} \left( \psi^* \sigma \otimes \frac{\partial \psi}{\partial x} \right),
\]

where \( \psi^* \) stands for the Hermitian conjugate of \( \psi \), \( \sigma \) is the Pauli matrix with components

\[
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},
\]

and we have chosen \( \hbar = 1, m = 1, \) as well as \( \sqrt{\Omega} = 1 \). We also chose \( k = 1 \) for the incident wavevector. The spin current \( Q \) in (2.35) is a rank 2 tensor, which contains the direction of both of the electron spin and wavevector.

From the continuity condition, the difference in spin current flowing into and out of the ferromagnet quantifies the rate of change of angular momentum, which allows us to write the spin transfer torque as

\[
\tau_{\text{STT}} = - \left( -\hat{x} \cdot Q |_{x = -\frac{w}{2}} + \hat{x} \cdot Q |_{x = -\frac{w}{2} + \lambda} \right),
\]

with \( \lambda = w \) (the width of the ferromagnet). More generally, (2.37) gives the rate of angular momentum transfer within the region \( x \in (-\frac{w}{2}, -\frac{w}{2} + \lambda) \) for arbitrary \( \lambda \geq 0 \).

Graphs in Fig. 2.18b show the transmitted and reflected electron current, the spin up and spin down components of the electron current, i.e., \( J_{\uparrow(\downarrow)} = \text{Im} \left( \psi^* \frac{\partial \psi_{\uparrow(\downarrow)}}{\partial x} \right) \), where \( \psi = \left( \psi_{\uparrow} \, \psi_{\downarrow} \right) \), the spin current \( Q \), and the spin transfer torque for \( \lambda \geq 0 \), for the case of a pure incident spin current with the spin direction defined by \( \theta = \pi/2 \). The kinetic energy of incident spins was chosen to be below the spin down potential barrier.
\( \left( \frac{k^2 \hbar^2}{2m} < V_\downarrow \right) \), by an amount expressed through \( \kappa_\downarrow = -ik_\downarrow \), where \( \frac{k^2 \hbar^2}{2m} = \frac{\nu^2 \hbar^2}{2m} - V_\downarrow \), or more simply, plugging in previously designated values for \( k \) and the constants, \( \kappa_\downarrow = \sqrt{2V_\downarrow - 1} \).

For \( \kappa_\downarrow = 0 \) (Fig. 2.18c), owing to partial reflection from the spin down barrier, the net electron current transmitted \( J_{\text{trans}} \) (purple line) through the ferromagnet (occupying space \( x \in (-w/2, w/2) \), where \( w = 2 \)) is reduced from the incident amplitude \( J_{\text{in}} = 1 \) by an amount \( J_{\text{refl}} \) corresponding to the reflected electron current given in Fig. 2.18b (purple line). The total incident (and transmitted) electron current, is equal to the sum of the amplitudes of the spin up and spin down current components. The amplitudes of the two current components are equal on incidence (due to \( \theta = \pi/2 \)), but differ for the transmitted and reflected currents due to the spin-dependent potential profile (Fig. 2.18a). Since the barrier is zero for spin up carriers, the reflected current has a large amplitude for the spin down component, whereas the transmitted current holds a greater amplitude for the spin up component. The \( z \)-component of the total spin current of the transmitted and reflected waves (see (2.35)) is described by the green line in Fig. 2.18b. Notice that the \( z \)-component of the reflected spin current is positive, despite electrons moving to the left. This is because reflected electrons are spin down, and a spin down electron moving to the left is equivalent to a spin up electron moving to the right in terms of spin current.

Graphs in Fig. 2.18c show all three components of the spin current for the incident wave, the transmitted wave, as well as the barrier region \( (-w/2 < x < w/2) \). An exclusive comparison of the incident and reflected spin currents for all three components is given in Fig. 2.18d (note the mirroring of the \( x \)-axis about \( x = 0 \)). The torque within the region \( -w/2 < x < w/2 + \lambda \), for \( \lambda \geq 0 \), as computed using (2.35), is shown in Fig. 2.18e. Passed the vertical green line (marking \( \lambda \) at which the entire ferromagnetic region is included in (2.37)), the spin torque saturates and is equal to the rate of net angular momentum transfer to the ferromagnet. The graphs show zero torque along the \( z \)-direction (direction of magnetization), and a non-vanishing torque in the perpendicular \( x \)- and \( y \)-directions. The resultant torque to the ferromagnet works to align its magnetization along the spin direction of the incoming electrons. The two components of the non-vanishing transverse spin torque are classified as in-plane (\( x \)-component in this case) and out-of-plane (\( y \)-component) contributions with respect to the plane defined by the incident spin direction and magnetization of the ferromagnet.

In a more realistic model regardful of the Fermi surface from which electrons are
incident, classical dephasing is shown to suppress the amount of transferred out-of-plane angular momentum [Ralph and Stiles, 2008]. Classical dephasing occurs because electrons of different incident energies ($k$) and approach angles ($\vartheta$) precess about the exchange field (direction of magnetization) at different frequencies ($\propto \Delta E \propto (k_{\uparrow} \cos \vartheta)^2 + (k_{\downarrow} \cos \vartheta)^2$, where $\vartheta = 0$ for trajectories normal to the NM/FM interface). Assuming full dephasing (often a valid assumption for all-metallic junctions), the in-plane component of the incident angular momentum is fully absorbed by the ferromagnet, and the quantity of absorbed out-of-plane angular momentum is zero. In magnetic tunnel junctions (MTJs), on the other hand, dephasing can be limited due to an appreciable probability of transmission exclusive to narrow regions of the Fermi surface [Theodonis et al., 2006]. Micromagnetic modeling of in-plane and out-of-plane torques in multilayer junctions is presented in section 4.1.2.

Lastly, we note that the transfer of angular momentum between a spin current and magnetization is also possible in continuous textured magnetic systems, such as a current carrying nanowire featuring a domain wall. In this case, the spatially varying magnetization may be regarded as a multilayer composed of infinitesimally thin layers, in a manner reflecting the system discussed earlier (Fig. 2.17), from which the spin transfer torque may be deduced [Thiaville et al., 2005]. To correctly capture details of the physics, considerations must be regardful of the degree to which length scales characterizing the geometry, in particular the layer thicknesses (in case of junctions) or the magnetization gradients (in case of domain walls), are comparable with length scales characterizing transport dynamics [Thiaville et al., 2005].

In conclusion, we have summarized the quantum mechanical origin of the spin transfer torque. Using a simple 1D toy model, following original work [Berger, 1996, Slonczewski, 1996], as well as [Ralph and Stiles, 2008], we have illustrated that a spin-dependent potential (representing a NM/FM/NM junction) can absorb angular momentum from itinerant spins. If the rate of absorption is sufficiently great to overcome dissipation due to damping, the magnetization of the ferromagnet can be destabilized from its original equilibrium position. Technological applications of spin transfer torques are discussed in chapter 12 and 13.
2.1.9 Interaction with Heat Bath

In this section we review the coupling of the magnetization to the heat bath. We will consider the situation when the spin subsystem is in thermal equilibrium with the lattice and electron subsystems. Nonequilibrium effects will be addressed in the subsequent two sections.

To begin our discussion, we consider a ferromagnetic system at zero temperature \( T = 0 \). The zero-temperature consideration is to be taken to mean absence of thermal fluctuations. This implies a deterministic magnetization response entirely due to interactions described in the preceding sections. These interactions act on the magnetization via effective magnetic fields or torques that predictably drive magnetization dynamics. For example, when the magnetization is collinear with the effective field throughout the magnetic body, and the net torque zero, the magnetization is perfectly stationary (no precession).

As temperature is increased, disorder is introduced to the system, and the once stationary magnetization now unpredictably fluctuates. If the temperature is not too high, the fluctuation at any point is around the local micromagnetic energy minimum (equilibrium configuration) defined by the deterministic interactions outlined earlier. At elevated temperatures, however, the magnetization may transition from the vicinity of one local minimum to the vicinity of another, due to large amplitude fluctuations. In bistable systems (see Fig. 2.6, for example), such fluctuations can result in what is known as thermally-induced reversal. The expectation time for thermally-induced transitions is expressed by the Arrhenius-Neé law

\[
\tau = \tau_0 \exp \left( \frac{\Delta E}{k_B T} \right),
\]

where \( \Delta E \) is the minimum energy barrier separating the two equilibrium states (see Fig. 2.7, for example), \( T \) is the temperature, \( f_0 = 1/\tau_0 \) is the attempt frequency (typically \( \sim 10^{10} \) Hz), and \( k_B \) is the Boltzmann constant.

We see that at higher temperatures the average wait time for a transition to occur is shorter, as anticipated due to larger amplitude fluctuations. The often observed high-incidence transitions between two stable states are known as telegraph noise [Cucchiara et al., 2009]. The expectation time for a transition is non-vanishing even for very low temperatures. This is due to the fact that the heat bath acts on the spin system through effective thermal fields that are randomly drawn from a Gaussian distribution whose
noise power, as determined from the fluctuation-dissipation theorem [Berkov, 2007], is

\[ D = \frac{\alpha}{1 + \alpha^2} \frac{k_B T}{\gamma \mu}. \]

(2.39)

Here, \( \alpha \) is the damping parameter, \( \gamma \) is the gyromagnetic ratio, and \( \mu \) is the magnetic moment magnitude on which the random thermal field is considered to act. Indeed, as the thermal field comes in the form of noise with some temperature-dependent power distribution, the probability that the random field strikes consequentially, even at low \( T \), is finite.

For this reason, careful consideration of energy barriers is necessary when designing magnetic memories and related devices. In hard-disk drives and magnetic random access memories (MRAM), at least 10 years of data retention (thermal stability) is desired, which, from equation (2.38), implies \( \Delta E \gtrsim 50 k_B T \), for \( T = 300 \text{ K} \). Since \( \Delta E \) is proportional to volume, the procedure for increasing information storage capacity by reducing the characteristic size of magnetic storage elements (i.e., by scaling down) runs into serious problems. Materials engineering plays a central role in providing sufficient thermal stability for reduced dimensions through enhancements in material properties, in particular magnetocrystalline anisotropy (section 2.1.3). However, while an increase in magnetic anisotropy ensures greater resistance to thermal fluctuations, it simultaneously degrades writability, i.e., the capability to reverse (switch) the magnetization state of an element encoding a bit. The struggle between thermal stability, writability, signal-to-noise ratio, reproducibility, and power consumption, kindled by scaling to ever-greater bit densities, thematically pervades much of part III of the present dissertation.
For the case of thermal equilibrium at some temperature $T$, the saturation magnetization (magnetic moment density) for a magnetic material is constant, and denoted by $M_s(T)$. Since elevated temperatures imply increased disorder, the magnetic moments on the atomic scale fluctuate with reduced cooperativeness at greater $T$, and the net moment density in continuum is seen as abated. Indeed, as $T$ approaches the Curie temperature ($T_C$), magnetization is effectively destroyed by thermal disorder. Figure 2.19 illustrates the disorder of magnetic moments on the atomic level when $T$ is near $T_C$. Notice that averaging over many spins yields near-zero net moment.

The magnetocrystalline anisotropy energy density $K(T)$ also falls off with temperature. This is because $K$ is determined by the spin-orbit interaction (section 2.1.3), i.e., coupling to the lattice potential, which itself is affected by disorder through phonon distributions.

The temperature dependence of material parameters just discussed, and the Arrhenius-Neél law of thermal activation covered earlier, have a direct bearing on MH loop measurements. Figure 2.20 illustrates the typical relationship between MH loops obtained at different temperatures. The temperature dependence of the anisotropy is reflected in the narrowing of the MH loops in the $H$-direction with increasing $T$, and the saturation magnetization dependence on $T$ is reflected in the shrinking of the MH loops along the $M$-direction.
Thermal activation effects, on the other hand, are clearly observed from the MH loop dependence on the sweep rate. Figure 2.21 illustrates the coercivity (the field amplitude at which $M = 0$ in the MH loop) as a function of the rate at which the applied field is swept during the MH loop measurement. For high sweep rates, the coercive field ($H_C$) is large, as thermal fluctuations are not allowed the ample time to significantly assist magnetization reconfiguration; see Eq. (2.38). The opposite is true for reduced sweep rates. Sharrock’s formula gives the relationship [Sharrock, 1994]

$$H_C = H_0 \left[ 1 - \frac{1}{a} \ln \left( \frac{f_0 H_0}{2a R} \right) \right],$$  

(2.40)

where $R$ is the sweep rate, $H_0$ is the short-time coercivity ($R \to \infty$), $f_0$ is the attempt frequency, $a = \frac{\Delta E_0}{k_B T}$, and $\Delta E_0$ denotes the barrier at zero bias. A similar expression holds for the threshold current required for switching the magnetization of a free layer via the spin transfer torque effect (section 2.1.8) in a spin valve (section 12.1.2). An applied field, and, in an effective manner, a spin-polarized current, can thus effect transitions from one stable state to another by lowering the associated energy barrier ($\Delta E$) and letting thermal activation do the rest (e.g., see Fig. 2.7). This is known as thermally assisted reversal in the presence of applied field and/or spin transfer torque. It is a matter of great technological implications, since in magnetic memories and related applications applied fields and currents must not exceed affordability thresholds, yet $\Delta E$ must be effectively reduced from a value corresponding to 10 years thermal stability at zero bias, to a barrier associated with an average transition time $\tau$ (Eq. (2.38)) on the order of 1 ns or less (required for high data rates). Furthermore, thermally assisted processes entail probability

**Figure 2.21:** Example of the dependence of coercivity on applied field sweep rate.
distributions which affect reproducibility, and must be well understood in order to be properly addressed. This is particularly important for achieving high performance and reliability in next-generation magnetic devices. More on thermal activation and thermally assisted reversal can be found in chapters 5, 6, 10, and 11.

Prior to closing, we note that the interaction between the spin system and the heat bath is responsible for magnetization damping; see (2.2) or (2.3). In other words, coupling of spins to the thermal reservoir allows the magnetization to approach alignment with the micromagnetic effective field and thus descend to a local minimum (micromagnetic equilibrium), as opposed to precessing indefinitely around the effective magnetic field at a fixed cone angle and energy (Fig. 2.1a). Damping therefore causes the moment vector to spiral in (relax) during precession towards the effective micromagnetic field (Fig. 2.1b), thereby reducing the cone angle and relieving some energy. This energy mostly goes to the lattice. Indeed, magnetization excitations, or magnon distributions, seek thermal equilibrium with the heat bath, and the damping parameter $\alpha$ in (2.2) reflects this coupling. See chapter 5 for more on thermal effects in micromagnetics.

### 2.1.10 Interaction with Heat Currents

A temperature gradient within a conductor provokes the flow of electrons from hot to cold. This is known as the Seebeck effect. Its inverse is the Peltier effect, describing the accumulation or depletion of heat at a metal/metal interface (thermocouple) due to a passing electric current. The spin degree of freedom adds a new dimension to thermoelectric effects. The study of coupling between spin, electron transport, and heat currents belongs to the field of spin caloritronics [Bauer et al., 2012].

Consider an externally sustained temperature gradient across a uniformly magnetized metallic ferromagnet. An electric current is expected to develop due to the Seebeck effect. However, since the conductor is ferromagnetic, the conductivity and Seebeck coefficients differ for the spin-up and spin-down carriers. The result is a net spin current [Uchida et al., 2008]. In a normal metal/ferromagnet (NM/FM) thermocouple, a maintained temperature difference across the interface can be used to drive spin injection into the normal metal. This is a manifestation of the so-called magneto-or spin-dependent Seebeck effect. Similarly, but in reverse chronology, a spin current injected into the ferromagnet is capable of driving a heat current across the NM/FM interface (spin-dependent Peltier effect).
Figure 2.22: Normal metal/ferromagnet insulator coupled structure with installed temperature gradient. A voltage develops across the normal metal in a direction normal to the temperature gradient.

Considering that the lattice, electron, and spin subsystems can all serve as conduits of heat, preclusion of the conduction electrons of the ferromagnet from participation in thermoelectric effects does not rule out spin caloritronic phenomena, in general. A sustained temperature gradient running through the interface of a normal metal/ferromagnet insulator (NM/IFM) coupled structure generates a voltage drop in the normal metal in a direction normal to the temperature gradient (Fig. 2.22). The voltage develops as a result of an injected spin current and a differential asymmetry in direction-dependent scattering probabilities for the two spin species in the normal metal (inverse spin Hall effect). The net spin current entering the normal metal is due to an imperfect compensation of incoming and outgoing spin currents conducted by thermal fluctuation-initiated spin pumping and spin-torque transfer processes [Bauer et al., 2012]. The former process evolves from spin-wave excitations, or thermally generated magnons, while the latter derives from Johnson-Nyquist noise in the normal metal. The spin current flowing into the normal metal exceeds the spin accumulation being injected counterward (per unit time) owing to the installed temperature bias. The noise-mediated mechanism is generally referred to as the spin Seebeck effect. It also operates in all-metallic devices, but we focused on the NM/IFM structure to accentuate the role of magnons as able carriers of heat. The inverse of the spin Seebeck effect is the spin Peltier effect. Neither is to be confused with a spin-dependent Seebeck or Peltier effects discussed earlier.

As has been illustrated, involvement of ferromagnets and the spin degree of freedom adds new flavor to thermoelectric effects. This includes the family of thermal
Hall effects [Goennenwein and Bauer, 2012]. The interaction between heat currents, charge carriers, and spins has important implications for device engineering at the nanoscale [Erekhinsky et al., 2012], where thermal torques can produce magnetization precession, lead to switching, induce domain wall motion, and result in a spin-wave Doppler shift, magnon-drag thermopower, and a nonadiabatic contribution to thermal spin transfer torque [Bauer et al., 2012]. The spin thermoelectric effects with their reciprocal relations are particularly attractive as a means of managing Joule heating in nanosized processing circuitry, and may provide a route toward efficient implementation of novel devices with new functionalities and modes of operation. A comprehensive overview of the field of spin caloritronics, including recent experimental and theoretical advances, can be found in [Bauer et al., 2012, Goennenwein and Bauer, 2012].

2.1.11 Interaction with Light

Another important interaction which enters the scope of micromagnetics is that between magnetization and light. This interaction has received significant research attention for the many curious phenomena it is responsible for and for the number of
prospective applications whose operation is based on it [Kirilyuk et al., 2010].

Consider a laser pulse incident on a magnetic material. The manner in which the light couples to the magnetization (spins) can greatly vary depending on the specifics of the irradiation and material systems involved. If the magnetic body is absorptive and the pulse long enough, light will transfer a significant amount of heat to the system, increasing its overall temperature, and inducing a change in system parameters (e.g., a reduction in anisotropy energy and saturation magnetization, see Fig. 2.23), thus influencing magnetization response. The interaction of light and magnetization on this level is exploited in heat assisted magnetic recording (HAMR) technology to achieve regions of increased writability in an otherwise highly incoercible medium (chapter 10).

In transparent materials, optical heating is inappreciable, and the light is seen to couple to the magnetization in a far more delicate manner than in the previous example. Faraday rotation and magneto-optic Kerr reflection describe phenomena where the propagating light undergoes a change in polarization due to interaction with the charge of the electric medium. The inverse Faraday effect, on the other hand, describes the change in magnetization induced by circularly polarized light. The effect is of great practical significance as it provides a means to optically control magnetization in select materials via an effective magnetic field $H_F \propto \mathbf{E} \times \mathbf{E}^*$. As seen from the expression, right and left circularly polarized waves occasion effective magnetic fields of opposite sign. The relation can be obtained by phenomenologically incorporating the electric field of light into the energy functional [Kirilyuk et al., 2010], or from microscopic considerations of a collisionless electron plasma [Hertel, 2006].

As light may couple to the magnetization in various ways, the effects of the interaction are generally classified as [Kirilyuk et al., 2010]: thermal, nonthermal photoabsorbing, and nonthermal non-photoabsorbing. Laser induced heating for use in HAMR, discussed at the beginning of this section, is an example of a thermal effect. More generally, the thermal effects category includes ultrafast magnetization processes in metallic ferromagnets, ferrimagnets, magnetic semiconductors, and other material systems, as well as phenomena such as heat-induced magnetic precession and switching. The nonthermal photoabsorbing effects include photoinduced changes to magnetocrystalline anisotropy, magnetization precession, and magnetization enhancement. The inverse Faraday effect, mentioned earlier, falls into the nonthermal non-photoabsorbing class of magneto-optic phenomena. A comprehensive review of the different effects and recent progress in the
field is given in [Kirilyuk et al., 2010].

2.2 Derivation of the Effective Field from the Variation of Energy

2.2.1 Variational Approach

Consider an energy functional in the general form

\[ E(\hat{m}) = \int_V \varepsilon(\hat{m}) dV, \]

(2.41)

where \( \varepsilon(\hat{m}) \) is the energy density and \( \hat{m} \) is the magnetization unit vector. We take the first order variation of \( E(\hat{m}) \) with respect to \( \hat{m} \) following Brown’s original approach [Brown, 1978]

\[ \delta E(\hat{m}) = \int_V \frac{\delta \varepsilon(\hat{m})}{\delta \hat{m}} \cdot \delta \hat{m} dV. \]

(2.42)

The variation in \( \hat{m} \) is arbitrary to the extent that \( |\hat{m} + \delta \hat{m}| = |\hat{m}| = 1 \), which corresponds to the necessary condition of unchanging saturation magnetization in the system in the absence of thermal effects. Hence, \( \delta \hat{m} \) can conveniently be written as

\[ \delta \hat{m} = \hat{m} \times \delta \theta, \]

(2.43)

where \( \delta \theta \) is an arbitrary infinitesimal rotation vector orthogonal to \( \hat{m} \). Plugging this into (2.42), and employing the vector identity \( a \cdot (b \times c) = -c \cdot (b \times a) \), we get

\[ \delta E(\hat{m}) = -\int_V \left( \hat{m} \times \frac{\delta \varepsilon(\hat{m})}{\delta \hat{m}} \right) \cdot \delta \theta dV. \]

(2.44)

Since \( \delta \theta \) in (2.44) is arbitrary up to the imposed constraint \( \hat{m} \cdot \delta \hat{m} = 0 \), then, in satisfaction of the equilibrium condition \( \delta E = 0 \), the following equation must hold

\[ \hat{m} \times \frac{\delta \varepsilon(\hat{m})}{\delta \hat{m}} = 0. \]

(2.45)

Rewriting the equilibrium condition as

\[ M \times \frac{\delta \varepsilon(M)}{\delta M} = 0, \]

(2.46)

where \( M = M_s \hat{m} \) is the magnetization, we can identify the magnetic field \( \mathbf{H}_{\delta V} \) originating from interaction energy \( E(M) \), and acting on an infinitesimal magnetic moment \( \delta \mu = \)
Figure 2.24: Infinitesimal volume $\delta V$ containing the magnetic moment with respect to which the energy is varied when (a) $\delta V$ is interior to an arbitrary magnetic body, and when (b) $\delta V$ is at the body boundary.

$M_{s,\delta V} \delta V \hat{m}_\delta V$ residing in an infinitesimal region $\delta V$ of the magnetic body, to be

$$H_{\delta V} = -\frac{1}{M_{s,\delta V} \delta V} \frac{\delta E(\hat{m})}{\delta \hat{m}_{\delta V}}.$$  \hspace{1cm} (2.47)

Here, $\frac{\delta E(\hat{m})}{\delta \hat{m}_{\delta V}}$ represents the rate of change of total system energy as $\hat{m}_{\delta V}$ is varied. It can be seen that the equilibrium condition $\delta E = 0 \iff \mathbf{M} \times \mathbf{H} = 0$ is only satisfied when $\mathbf{M} \parallel \mathbf{H}$ throughout the system, in agreement with our discussion in the preamble to section 2.1. When a system is displaced from equilibrium, the field $\mathbf{H}$ drives system dynamics according to the LLG equation (2.3), which involves precession of $\mathbf{M}$ about $\mathbf{H}$, as well as magnetization damping toward an equilibrium configuration for which $\mathbf{M} \parallel \mathbf{H}$.

Notice that in (2.45) (and hence in (2.47)), the variation of the energy with respect to the magnetization unit vector need not be constrained, as the cross product with $\hat{m}$ in (2.45) (as well as in the LLG equation (2.3)) automatically orthogonalizes the torque with respect to $\hat{m}$, thus implicitly ensuring the preservation of magnetization magnitude.

2.2.2 Bulk Exchange Field

The bulk exchange energy was given in section 2.1.6 as

$$E_{\text{ex}} = \int_V A(\nabla \hat{m})^2 dV.$$  \hspace{1cm} (2.48)
In view of (2.47), the bulk exchange field can be written as

$$H_{\text{ex}, \delta V} = -\frac{1}{M_s, \delta V} \frac{\delta E_{\text{ex}}}{\delta \hat{m}_{\delta V}} = -\frac{1}{M_s, \delta V} \frac{1}{\delta \hat{m}_{\delta V}} \int_V 2A \nabla \hat{m} (\delta \nabla \hat{m}) dV .$$  \hspace{1cm} (2.49)

Using the identity

$$\nabla \hat{m} \cdot \delta \nabla \hat{m} = \nabla \hat{m} \cdot \nabla \delta \hat{m} = -\delta \hat{m} \nabla^2 \hat{m} + \nabla \cdot (\delta \hat{m} \nabla \hat{m})$$

and applying Gauss's theorem, we obtain

$$H_{\text{ex}, \delta V} = \frac{1}{M_s, \delta V} \frac{1}{\delta \hat{m}_{\delta V}} \left( \int_V 2A (\delta \hat{m} \nabla^2 \hat{m}) dV - \oint_S 2A \delta \hat{m} (\nabla \hat{m} \cdot \hat{n}) dS \right) ,$$  \hspace{1cm} (2.50)

where $\hat{n}$ is the outward unit normal to surface $S$ bounding volume $V$.

If the variation of the energy is with respect to the moment within an infinitesimal region $\delta V$ interior to $V$ and away from the boundary surface $S$ (Fig. 2.24a), then the surface integral in (2.50) vanishes, as we are not varying $\delta \hat{m}$ along the boundary to $V$. Furthermore, the integration over $V$ in this case reduces to an integration over $\delta V$, as we are varying the moment only within the region $\delta V$. Since $\delta V$ is infinitesimal, we have that $\int_{\delta V} (\ )dV \to (\ )\delta V$, and after cancelation, we arrive at

$$H_{\text{ex}, \delta V} = \frac{2A_{\delta V}}{M_s, \delta V} \nabla^2 \hat{m} \bigg|_{\delta V} \ (\text{interior}) .$$  \hspace{1cm} (2.51)

Conversely, when $\delta V$ lies along the boundary $S$ (Fig. 2.24b), we have $\int_{\delta V} (\ )dV \to (\ )\delta V$ and $\int_{\delta S} (\ )dS \to (\ )\delta S$, and thus

$$H_{\text{ex}, \delta V} = \frac{2A_{\delta V}}{M_s, \delta V} \nabla^2 \hat{m} \bigg|_{\delta V} - \frac{2A_{\delta V}}{M_s, \delta V} \frac{1}{\delta t} \frac{\partial \hat{m}}{\partial \hat{n}} \bigg|_{\delta S} \ (\text{at boundary}) ,$$  \hspace{1cm} (2.52)

where $\nabla_\parallel = \nabla - \nabla_\perp$,

$$\frac{\partial \hat{m}}{\partial \hat{n}} = \nabla_\perp \hat{m} = \nabla \hat{m} \cdot \hat{n} ,$$  \hspace{1cm} (2.53)

and

$$\delta t = \frac{\delta S}{\delta V} .$$  \hspace{1cm} (2.54)

We note that $\delta S$ represents the infinitesimal surface belonging to $S$, and not the entire bounding surface enclosing $\delta V$.

The surface term in (2.52) is the exchange field contribution that acts on the magnetic moment extending from the bounding surface a thickness $\delta t$ into the volume, in the limit $\delta t \to 0$. This surface term together with the appearance of the parallel gradient $\nabla_\parallel$ in (2.52) reflects the condition of disrupted bulk exchange due to the inherent discontinuity at the body boundary (Fig. 2.24). The infinitesimal quantity $\delta t$ appearing in the surface term assumes a finite value in finite element modeling, where the magnetic system is spatially discretized, as shown in chapter 3.
2.2.3 Interlayer Exchange Field

From (2.23), the interlayer exchange functional is

\[ E_{\text{ex}} = - \int_S J \hat{\mathbf{m}}_+ \cdot \hat{\mathbf{m}}_- dS, \]  

(2.55)

where indices + and − denote the two coupled surfaces, respectively (Fig. 2.25). To obtain the field acting on the moment belonging to an infinitesimal volume \( \delta V_+ \) lying along surface (+), we employ (2.15). This gives

\[ H_{\text{ex}, \delta V_+} = - \frac{1}{M_s \delta V_+} \frac{\delta E_{\text{ex}}}{\delta \hat{\mathbf{m}}_+} = \frac{1}{M_s \delta V_+} \frac{1}{\delta V_+} \int_S J \hat{\mathbf{m}}_+ \cdot \hat{\mathbf{m}}_- dS. \]  

(2.56)

On behalf of the local variation in \( \hat{\mathbf{m}}_{\delta V_+} \), only integration over \( \delta S \) yields a contribution. Using \( \int_{\delta S} ( \ ) dS \rightarrow ( \ ) \delta S \), the above expression can be simplified to

\[ H_{\text{ex}, \delta V_+} = \frac{J \delta S_+}{M_s \delta V_+ \delta t_+} \hat{\mathbf{m}}_{\delta V_+}. \]  

(2.57)

The field \( H_{\text{ex}, \delta V_+} \) acts on the magnetic moment within volume \( \delta V_+ \) lying along surface (+) extending a thickness \( \delta t_+ \) into the magnetic body, in the limit \( \delta t_+ \rightarrow 0 \) (Fig. 2.25). In the finite element representation of chapter 3, \( \delta t_+ \) takes on a finite value.
2.2.4 Bulk Anisotropy Field

For the case of bulk magnetocrystalline uniaxial anisotropy (section 2.1.3), the energy functional is

\[ E_{\text{anis}} = - \int_V K(\hat{m} \cdot \hat{k})^2 dV. \tag{2.58} \]

Using (2.47), we obtain the corresponding anisotropy field

\[ H_{\text{anis},\delta V} = - \frac{1}{M_{s,\delta V}} \frac{\delta E_{\text{anis}}}{\delta \hat{m}_{\delta V}} = \frac{1}{M_{s,\delta V}} \frac{1}{\delta V} \frac{1}{\delta \hat{m}_{\delta V}} \int_V 2K(\hat{m} \cdot \hat{k})\hat{k} \cdot \delta \hat{m} dV. \tag{2.59} \]

Since the magnetocrystalline interaction is local in character, the integration region can be reduced to an infinitesimal domain, so that \( \int_{\delta V} (\ )dV \to (\ )\delta V \), as the variation is confined to \( \hat{m} \) within \( \delta V \). Therefore, after cancelation, we have

\[ H_{\text{anis},\delta V} = \frac{2K_{\delta V}}{M_{s,\delta V}} (\hat{m}_{\delta V} \cdot \hat{k}_{\delta V})\hat{k}_{\delta V}. \tag{2.60} \]

2.2.5 Surface Anisotropy Field

Restricting consideration to uniaxial surface (or interface) anisotropy, the energy density is

\[ E_{\text{anis}}^s = - \int_S K^s(\hat{m} \cdot \hat{k}^s)^2 dS, \tag{2.61} \]

where \( K^s \text{ (erg/cm}^2\text{)} \) is the anisotropy energy density per unit surface area. The associated field is

\[ H_{\text{anis},\delta V}^s = - \frac{1}{M_{s,\delta V}} \frac{\delta E_{\text{anis}}^s}{\delta \hat{m}_{\delta V}} = \frac{1}{M_{s,\delta V}} \frac{1}{\delta V} \frac{1}{\delta \hat{m}_{\delta V}} \int_S 2K^s(\hat{m} \cdot \hat{k}^s) \cdot \hat{k}^s \delta \hat{m} dS. \tag{2.62} \]

Due to the local variation in \( \hat{m} \delta V \), we have \( \int_{\delta S} (\ )dS \to (\ )\delta S \), so that

\[ H_{\text{anis},\delta V}^s = \frac{1}{\delta t} \frac{2K_{\delta V}^s}{M_{s,\delta V}} (\hat{m}_{\delta V} \cdot \hat{k}_{\delta V}^s)\hat{k}_{\delta V}^s, \tag{2.63} \]

where \( \delta t = \delta S/\delta V \) (Fig. 2.24). This field acts on the magnetic moment within \( \delta V \) extending from the surface a thickness \( \delta t \) into the magnetic body, in the limit \( \delta t \to 0 \). In finite element micromagnetic modeling, the quantity \( \delta t \) takes on a finite value, as will be shown in chapter 3.
2.2.6 Magnetostatic Field

The magnetostatic field is the stray field produced by the magnetization $\mathbf{M}$. Its expression from section 2.1.2 is

$$
\mathbf{H}_{\text{ms}}(\mathbf{r}) = \nabla \int \frac{\nabla' \cdot \mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, dV' - \nabla \oint \frac{\hat{n} \cdot \mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, dS'.
$$

(2.64)

2.2.7 Zeeman Field

The Zeeman field is the magnetic field that is applied externally on a sample,

$$
\mathbf{H}_{\text{Zee}}(\mathbf{r}) = \mathbf{H}_{\text{a}}(\mathbf{r}),
$$

(2.65)

and, as such, is typically known in advance.

2.2.8 The Effective Field

The effective field which enters the LLG equation (2.3), the governing equation of field-driven magnetization dynamics, is the sum of all fields originating from interactions that can be represented by an energy functional $E_{\text{int}}(\mathbf{\hat{m}})$. For the case of a system involving interactions discussed in sections 2.2.2–2.2.7, the effective field is

$$
\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{Zee}} + \mathbf{H}_{\text{ms}} + \mathbf{H}_{\text{anis}}^\theta + \mathbf{H}_{\text{anis}}^\rho + \mathbf{H}_{\text{ex}} + \mathbf{H}_{\text{iex}}.
$$

(2.66)

The effective field drives the magnetization into dynamics when displaced from equilibrium. Brown’s equations are just the equilibrium condition $\mathbf{\hat{m}} \times \mathbf{H}_{\text{eff}} = 0$ (see (2.46)) separated into two expressions, one involving the volume contributions to the field, namely, $\mathbf{H}_{\text{Zee}}$, $\mathbf{H}_{\text{ms}}$, $\mathbf{H}_{\text{anis}}$, and the volume contribution of bulk exchange $\mathbf{H}_{\text{ex}}$, as given by (2.51) or the first term in (2.52), and the other involving the surface contributions to the field, i.e., $\mathbf{H}_{\text{anis}}^\rho$, $\mathbf{H}_{\text{iex}}$, and the surface contribution of $\mathbf{H}_{\text{ex}}$ (second term in (2.52)). When surface anisotropy and interlayer exchange are absent, the only surface contribution is that from the second term in (2.52), in which case the second expression in Brown’s equations takes the form

$$
\mathbf{\hat{m}} \times \frac{\partial \mathbf{\hat{m}}}{\partial \hat{n}} = 0,
$$

(2.67)

or better yet [Brown, 1978]

$$
\frac{\partial \mathbf{\hat{m}}}{\partial \hat{n}} = 0,
$$

(2.68)

as any change in $\mathbf{\hat{m}}$, including $\frac{\partial \mathbf{\hat{m}}}{\partial \hat{n}}$, must be orthogonal to $\mathbf{\hat{m}}$, in accordance with the premised constancy of the magnetic moment density, $|\mathbf{\hat{m}}| = 1$. 
Part II

Micromagnetic Modeling
This chapter describes finite element modeling using the linear basis representation. Micromagnetic fields are expressed in discretized form following the procedure in [Chang et al., 2011]. The correspondence between infinitesimal quantities in continuum micromagnetics and finite quantities in finite element modeling is established. Subtleties involving indirect exchange coupling across a nonmagnetic spacer layer are discussed. The subject matter covered in this chapter is the basis for micromagnetic finite element modeling of spin transfer torques and thermal effects presented in the subsequent two chapters. The modeling forms the general computational framework for many of the simulation studies presented in part III of this dissertation.

### 3.1 Finite Element Representation

Micromagnetic modeling is a powerful tool for investigating magnetization behavior in a wide range of magnetic systems [Scheinfein, 1997, Donahue and Porter, 1999, Suess et al., 2002, Scholz et al., 2003, Chang et al., 2011]. Consider as an example a complex system involving a magnetic recording head located over exchange coupled composite bit patterned media, as illustrated in Fig. 3.1. The first step in solving for the magnetization dynamics of such systems is to discretize all volumes into finite elements. We consider a tetrahedral discretization scheme where the unit magnetization vector \( \hat{m} \) is prescribed at the mesh nodes (tetrahedral vertices) (Fig. 3.2). We wish \( \hat{m} \) to be a continuous function defined throughout the magnetic volume, not just at the mesh nodes, to comply with the continuum hypothesis of micromagnetics on which we shall base our modeling. The unit magnetization vector \( \hat{m} \) will be continuously defined throughout all volumes once
\( \hat{\mathbf{m}}^l(\mathbf{r}) \) is defined within each tetrahedron \( l \). We represent \( \hat{\mathbf{m}} \) within the volume of each tetrahedron using

\[
\hat{\mathbf{m}}^l(\mathbf{r}) = \sum_{k=1}^{4} \hat{\mathbf{m}}_k^l \xi_k^l(\mathbf{r}), \tag{3.1}
\]

where \( \hat{\mathbf{m}}_k^l \) is the magnetization unit vector defined at each of the four vertices of tetrahedron \( l \), and \( \xi_k^l(\mathbf{r}) \) is a hat basis function which equals to unity at vertex \( k \), linearly tapers off to zero at the opposite tetrahedral face, and remains zero exterior to the tetrahedron. This is known as the linear basis representation. We simulate magnetization dynamics by evolving the magnetization unit vector defined on global node \( p \), for all nodes \( p \) of the mesh, according to the Landau-Lifshitz-Gilbert (LLG) equation (2.3) in discretized form,

\[
\frac{d\hat{\mathbf{m}}_p}{dt} = -\frac{\gamma}{1 + \alpha_p^2} \hat{\mathbf{m}}_p \times \mathbf{H}^{\text{eff}}_p - \frac{\gamma \alpha_p}{1 + \alpha_p^2} \hat{\mathbf{m}}_p \times \hat{\mathbf{m}}_p \times \mathbf{H}^{\text{eff}}_p, \tag{3.2}
\]

with \( \mathbf{H}^{\text{eff}}_p \) being the effective field at node \( p \). For a particular tetrahedron, the action of the effective field at the four tetrahedral vertices, in the linear basis formulation, has an accumulative effect on the magnetic moment throughout the tetrahedron. In order to simulate dynamics, it is important to correctly map the previously obtained interaction fields (section 2.2.8) acting on the magnetic moment throughout the magnetic body to

**Figure 3.1**: Magnetic recording head situated over patterned media: (a) model geometry; (b) zoom-in showing discretized pole tip and composite patterned islands; (c) \( z \)-component of magnetization at an instant of simulation (red represents the \( +z \) magnetization direction, blue represents the \( -z \) magnetization direction).
Figure 3.2: Typical tetrahedral discretization element (indexed $l$) showing four nodal vectors from which the magnetization direction throughout the tetrahedron is expanded using linear basis functions.

the effective field $H_p^{\text{eff}}$ at each node $p$ of the discretized system. Alternatively, one can derive $H_p^{\text{eff}}$ from the variation of the total system energy cast in discretized form with respect to $\mathbf{m}_p$.

3.2 Calculation of the Micromagnetic Fields at the Mesh Nodes

3.2.1 Bulk Exchange Field

The expression for the bulk exchange contribution to the effective field, derived in section 2.2.2, is

$$H_{\text{ex},\delta V}^{\text{bulk}} = \frac{2A_{\delta V}}{M_s,\delta V} \nabla^2 \mathbf{m}_{\delta V} \bigg|_{\text{interior}},$$

(3.3)

$$H_{\text{ex},\delta V}^{\text{bulk}} = \frac{2A_{\delta V}}{M_s,\delta V} \left( \nabla_{\parallel}^2 \mathbf{m} \bigg|_{\delta V} - \frac{1}{\delta t} \frac{\partial \mathbf{m}}{\partial \mathbf{n}} \bigg|_{\delta S} \right) \bigg|_{\text{at boundary}}.$$  

(3.4)

The bulk exchange field expressed in continuum form (3.3) and (3.4) has the finite element representation

$$H_{\text{ex},p}^{\text{bulk}} = \frac{2A_p}{M_{s,p}} \nabla^2 \mathbf{m}_{p} \bigg|_{\text{interior}},$$

(3.5)

$$H_{\text{ex},p}^{\text{bulk}} = \frac{2A_p}{M_{s,p}} \left( \nabla_{\parallel}^2 \mathbf{m} \bigg|_{p} - \frac{1}{t_p} \frac{\partial \mathbf{m}}{\partial \mathbf{n}} \bigg|_{p} \right) \bigg|_{\text{at boundary}}.$$  

(3.6)
Figure 3.3: 2D representation of a tetrahedral mesh. Tetrahedrons $k$ and $l$ are shaded to indicate connectivity and notation selected for denoting nodal magnetization unit vectors. Material properties are assumed uniform within each tetrahedron.

where $M_{s,p}$ represents the saturation magnetization associated with an effective volume $V_p$ belonging to node $p$ of the tetrahedral mesh representing the magnetic body, $A_p$ represents the effective exchange stiffness, $t_p$ accounts for the effective depth associated with node $p$ in the case that it is a boundary node, and $\hat{\mathbf{m}}$ is the magnetization unit vector to be expanded in terms of linear vector basis functions.

The explicit expressions for $\hat{\mathbf{m}}(\mathbf{r})$, $M_{s,p}$, $A_p$, and $V_p$ are

$$\hat{\mathbf{m}} = \sum_{l=1}^{M} \sum_{k=1}^{4} \xi^i_l \hat{\mathbf{m}}^i_k,$$  \hspace{1cm} (3.7)

$$M_{s,p} = \sum_{l=1}^{M} \int M_{s,p}^l \xi^i_l(p) \, dV = \frac{\sum_{l=1}^{M} A^l_{s,p} V^l}{\sum_{l=1}^{M} V^l},$$ \hspace{1cm} (3.8)

$$A_p = \sum_{l=1}^{M} \int A^l_{s,p} \xi^i_l \, dV = \frac{\sum_{l=1}^{M} A^l V^l}{\sum_{l=1}^{M} V^l},$$ \hspace{1cm} (3.9)

$$V_p = \sum_{l=1}^{M} \int \xi^i_l \, dV = \frac{1}{4} \sum_{l=1}^{M} V^l.$$ \hspace{1cm} (3.10)

In (3.7), $l$ runs over all $M$ tetrahedrons of the discretized system, and $k$ runs over the four vertices associated with each of the $M$ tetrahedrons. In (3.8)–(3.10), $l$ goes over only
the $M_p$ tetrahedrons that have node $p$ for a common vertex (Fig. 3.3). The notation $\xi_l(p)$ in (3.8)–(3.10) is used to represent the linear basis function associated with tetrahedron $l$ and global node $p$, and equals zero if global node $p$ is not a vertex of tetrahedron $l$. It was assumed that for each tetrahedron $l$ the values $M_s^l$ and $A_p^l$ are constant (Fig. 3.3). The expressions for $M_s^p$ and $A_p$ at node $p$ are recognized to be weighted averages over surrounding tetrahedrons, while $V_p$ is the volume associated with node $p$, leading to the volumetric consistency condition $\sum_{i=1}^{N} V_p = V$, where $N$ is the total number of mesh nodes of the discretized system and $V$ is the total volume. In (3.8)–(3.10), use was made of the identity [Peterson et al., 1998]
\[
\int \xi_l \, dV = \frac{V^l}{4}.
\] (3.11)

Continuing with the derivation of the bulk exchange field at node $p$, and reflecting on equation (3.5) and (3.6), we observe that in the linear basis representation the second order derivative of $\hat{\mathbf{m}}(\mathbf{r})$ is zero everywhere except at the nodes, where $\nabla^2 \hat{\mathbf{m}}$ is singular. In order to calculate $\nabla^2 \hat{\mathbf{m}}|_p$ we begin by considering the following transformation
\[
b\nabla^2 \hat{\mathbf{m}} = \nabla \cdot (b\nabla \hat{\mathbf{m}}) - \nabla b \cdot \nabla \hat{\mathbf{m}},
\] (3.12)
which, upon integration and the application of Gauss’s theorem, yields
\[
\int_{V_p} b\nabla^2 \hat{\mathbf{m}} \, dV = - \int_{V_p} \nabla b \cdot \nabla \hat{\mathbf{m}} \, dV + \int_{S_p} b\nabla \hat{\mathbf{m}} \cdot \hat{n} \, dS.
\] (3.13)
Here, the volumetric integration region $V_p$, its boundary surface $S_p$, and the scalar function $b$ are arbitrary. To extract an explicit expression for $\nabla^2 \hat{\mathbf{m}}|_p$, we chose $b$ to equal $\xi_p^l$, and chose $V_p$ to comprise the volume of all tetrahedra that have node $p$ for a common vertex. Breaking up the integration domain into its tetrahedral parts, we obtain
\[
\sum_{l=1}^{M_p} \int_{\Gamma_l^l} \xi_l(p) \nabla^2 \hat{\mathbf{m}} \, dV = - \sum_{l=1}^{M_p} \int_{\Gamma_l^l} \nabla \xi_l(p) \cdot \nabla \hat{\mathbf{m}} \, dV + \sum_{l=1}^{M_p} \int_{\Omega_{\hat{n}}^l} \xi_l(p) \nabla \hat{\mathbf{m}} \cdot \hat{n} \, dS,
\] (3.14)
where $\Gamma_l^l$ and $\Omega_{\hat{n}}^l$ represent the volume and surface region of tetrahedron $l$ for all $M_p$ tetrahedrons comprising the volume $V_p$. Note that on account of the local nature of the linear basis functions, we may replace $\sum_{l=1}^{M_p}$ with $\sum_{l=1}^{M}$. Expanding $\hat{\mathbf{m}}$ in terms of the linear basis functions, we get
\[
\nabla^2 \hat{\mathbf{m}}|_p \sum_{l=1}^{M} \int_{\Gamma_l^l} \xi_l(p) \, dV = - \sum_{l=1}^{M} \int_{\Gamma_l^l} \nabla \xi_l(p) \cdot \nabla \left(\sum_{k=1}^{4} \hat{\mathbf{m}}^l_{k,k} \xi_l\right) \, dV
\]
\[
+ \sum_{l=1}^{M} \int_{\Omega_{\hat{n}}^l} \xi_l(p) \nabla \left(\sum_{k=1}^{4} \hat{\mathbf{m}}^l_{k,k} \xi_l\right) \cdot \hat{n} \, dS.
\] (3.15)
It was assumed that $\nabla^2 \hat{m}$ is slowly varying within the integration region so that it can be taken out of the integral. This approximation is reasonable provided that the mesh size is smaller than the exchange lengths characterizing magnetization texture, which typically are $l_{\text{ex}}^{\text{ms}} \approx \sqrt{A/(2\pi M_{s}^2)}$ and $l_{\text{ex}}^{\text{anis}} \approx \sqrt{A/K}$. Here, $M_s$, $A$, and $K$ are the saturation magnetization, exchange stiffness constant, and anisotropy energy density, respectively. A discussion of mesh criteria in the presence of spin transfer torques and thermal effects can be found in chapters 4 and 5.

The surface integral in equation (3.15) for a node $p$ interior to the surface boundary of the body vanishes due to the fact that the function $\xi_l(p)$ tapers off to zero at the tetrahedral face opposite to node $p$, leaving us with

$$\nabla^2 \hat{m}|_p = -\frac{1}{V_p} \sum_{l=1}^{M} \int_{\Gamma_l^i} \nabla \xi_l^i(p) \cdot \nabla \left( \sum_{k=1}^{4} \hat{m}_l^k \xi_l^k \right) dV \quad \text{(interior).} \quad (3.16)$$

In the derivation, use was made of identity (3.11). Finally, the bulk exchange field at interior node $p$ is

$$\mathbf{H}_{\text{ex},p}^{\text{bulk}} = \frac{2A_p}{M_{s,p}} \nabla^2 \hat{m}|_p = -\frac{2A_p}{M_{s,p}V_p} \sum_{l=1}^{M} \sum_{k=1}^{4} \hat{m}_l^k \int_{\Gamma_l^i} \nabla \xi_l^i \cdot \nabla \xi_l^k dV \quad . \quad (3.17)$$

We note that the gradient operator bypasses $\hat{m}_l^k$, since it is a nodal coefficient vector with no spatial dependence. Owing to the same reason, the dot product in the integrand above is between the two gradients of the hat basis functions and does not involve the nodal coefficient vector. Similarly, $\hat{m}_l^k$ need not be within the integrand. Recognizing that the gradient of a scalar function is a vector pointing in the direction of greatest ascent, whose magnitude reflects the rate of ascent, and bearing in mind that the hat basis function associated with node $q$ of tetrahedron $l$ equals unity at the node, and linearly tapers off to zero at the opposing tetrahedral face, we can, on geometrical grounds, formulate a general expression for the gradient of the hat basis function appearing in (3.17) as

$$\nabla \xi_l^q = \frac{\mathbf{p}_q^l}{|\mathbf{p}_q^l|^2} \quad . \quad (3.18)$$

The vector $\mathbf{p}_q^l$ points to node $q$ from a point belonging to the plane defined by the opposing tetrahedral face such that $\mathbf{p}_q^l$ is perpendicular to that plane (Fig. 3.4). In terms of the position vectors $\mathbf{r}_q^l$, $\mathbf{r}_r^l$, $\mathbf{r}_s^l$ and $\mathbf{r}_t^l$ of the four nodes of tetrahedron $l$, $\mathbf{p}_q^l$ is expressed as

$$\mathbf{p}_q^l = \left[ (\mathbf{r}_q^l - \mathbf{r}_r^l) \cdot \hat{\mathbf{n}}_r^l \right] \hat{\mathbf{n}}_{rst}^l \quad , \quad (3.19)$$
Figure 3.4: Vector $p^l_q$ extending from plane $rst$ to vertex $q$, appearing in (3.18).

where

$$
\hat{n}^l_{rst} = \frac{(r^l_r - r^l_s) \times (r^l_l - r^l_t)}{|(r^l_r - r^l_s) \times (r^l_l - r^l_t)|}.
$$

Expression (3.20) can be deduced from the expression for the volume of the tetrahedron

$$
V = \frac{1}{6} (r^l_r - r^l_s) \cdot [(r^l_r - r^l_s) \times (r^l_l - r^l_t)] = \frac{1}{3}Ah,
$$

where $A$ is the area of one of the three tetrahedral faces and $h$ is the height from that face to the opposing tetrahedral vertex (e.g.,

$$
A = \frac{1}{2} |(r^l_r - r^l_s) \times (r^l_l - r^l_t)| \quad \text{and} \quad h = (r^l_q - r^l_l) \cdot \frac{(r^l_r - r^l_s) \times (r^l_l - r^l_t)}{|(r^l_r - r^l_s) \times (r^l_l - r^l_t)|}.
$$

Expression (3.19) has the same form for all permutations of $(q,r,s,t)$. This can be seen by recognizing that

$$
a \text{ sign change in } \hat{n}^l_{rst} \text{ resulting from an odd permutation in } (r,s,t) \text{ does not arise in } p^l_q, \text{ owing to the double product with } \hat{n}^l_{rst}. \text{ Consequently, } p^l_q, \text{ as given in expression (3.19), always extends normally onto vertex } q \text{ from the plane defined by the opposing tetrahedral face, and thus is correctly in the direction of the gradient of the hat basis function } \nabla \xi^l_q, \text{ independent of node arrangement } (q,r,s,t). \text{ Since the integrand of the volume integral in (3.17) is constant, the bulk exchange field at interior node } p \text{ can be concisely written as}
$$

$$
\mathbf{H}^{\text{bulk}}_{\text{ex, } p} = \frac{2A_p}{M_{s.p}} \sum_{l=1}^{M} \sum_{k=1}^{4} \Lambda^{l}_{(p)k} \hat{n}^l_k \quad \text{(at interior node),}
$$

where

$$
\Lambda^{l}_{(p)k} = -\frac{V^l}{V_p} \nabla \xi^l_{(p)} \cdot \nabla \xi^l_k
$$

is a geometric factor reflecting the contribution of $\hat{n}^l_k$ at node $k$ of tetrahedron $l$ to the
exchange field at node \( p \) in terms of tetrahedral dimensions. More generally,

\[
\Lambda = \begin{pmatrix}
\Lambda_{11} & \cdots & \Lambda_{1N} \\
\vdots & \ddots & \vdots \\
\Lambda_{N1} & \cdots & \Lambda_{NN}
\end{pmatrix}
\] (3.23)

represents the Laplacian matrix operator, whose elements can be obtained as

\[
\Lambda_{mn} = \sum_{l=1}^{M} \sum_{k=1}^{4} \Lambda^l_{(m)k} \delta^l_{(n)k},
\] (3.24)

with \( \Lambda^l_{(m)k} \) given by (3.22), and \( \delta^l_{(n)k} = 1 \) if global node \( n \) coincides with node \( k \) of tetrahedron \( l \), and is zero otherwise. We note that the Laplacian operator \( \nabla^2 \) operates locally, meaning that \( \Lambda \) is a sparse matrix with the majority of elements identically equal to zero, thus urging the use of sparse matrix representation [Chang et al., 2011] to facilitate rapid computations (section 8.3).

Returning to the derivation of the bulk exchange field, we now consider the second case, when node \( p \) sits on the bounding surface \( S \) of the magnetic body. The surface integral in (3.15) has a non-vanishing component over the integration region belonging to the bounding surface, because there \( \xi^l_{(p)} \) is finite. Hence, for node \( p \) at the boundary, we have

\[
\nabla^2 \| \hat{m} \bigg|_p = -\frac{1}{V_p} \sum_{l=1}^{M} \int_{\Gamma_l} \nabla \xi^l_{(p)} \cdot \nabla \left( \sum_{k=1}^{4} \hat{m}^l_k \xi^l_{k} \right) dV \\
+ \frac{1}{V_p} \sum_{l=1}^{M} \int_{\Omega^l_{\hat{n}}} \xi^l_{(p)} \nabla \left( \sum_{m} \hat{m}^l_m \xi^l_{m} \right) \cdot \hat{n} dS \quad \text{(at boundary)},
\] (3.25)

where \( \nabla^2 = \nabla^2 - \nabla^2_\perp \), and \( m \) runs over boundary nodes only, which comprise the tetrahedral faces (integration domain \( \Omega^l_{\hat{n}} \)) laying on the bounding surface of the magnetic body having unit normal \( \hat{n} \). Since the second term on the right-hand side of (3.25) is recognized to be the finite element representation of \( \partial \hat{m} / \partial \hat{n} \bigg|_p \), taking it to the left-hand side and multiplying both sides of the equation by \( 2A_p/M_{s,p} \), we obtain the bulk exchange field at the boundary node \( p \)

\[
H^\text{bulk}_{ex,p} = \frac{2A_p}{M_{s,p}} \left( \nabla^2 \| \hat{m} - \frac{1}{t_p} \partial \hat{m} / \partial \hat{n} \right) \bigg|_p = \frac{2A_p}{M_{s,p}} \sum_{i=1}^{M} \sum_{k=1}^{4} \Lambda^l_{(p)k} \hat{m}^l_k \quad \text{(at boundary)},
\] (3.26)

which is identical to the expression obtained for the bulk exchange field at an interior node (3.21). The only difference is that the sum in (3.26) is a truncated sum in the sense
that the tetrahedra over which the sum runs do not enclose node \( p \), as is the case in (3.21). Therefore, the bulk exchange field on node \( p \) assumes the common form

\[
\mathbf{H}_{\text{ex},p}^{\text{bulk}} = \frac{2A_p}{M_{s,p}} \sum_{l=1}^{M} \sum_{k=1}^{A_l} \Lambda_{p,k} \hat{m}_l \text{ (general expression)},
\]

(3.27)

for all nodes \( p \), be they interior to the volume or on the body boundary.

Despite the common expression for the bulk exchange (3.27), which is valid for interior and surface nodes alike, and which we shall use in computation, it is insightful to obtain an expression for \( t_p \), as this is the finite element quantity corresponding the infinitesimal thickness \( \delta t \) (see (2.52)) marking the quantity of magnetic moment extending from the surface into the volume, in the limit \( \delta t \to 0 \), on which the surface contribution to the exchange field exerts a torque. One way to obtain \( t_p \) is to extract it from (3.25) or (3.26), from which we have

\[
\frac{1}{t_p} \frac{\partial \hat{m}}{\partial \hat{n}} \bigg|_p = \frac{1}{V_p} \sum_{l=1}^{M} \int_{\Omega^l_{\hat{n}}} \nabla \left( \sum_{m} \hat{m}_{l,m} \xi^l_{m} \right) \cdot \hat{n} \, dS.
\]

(3.28)

This can be simplified to

\[
\frac{1}{t_p} \frac{\partial \hat{m}}{\partial \hat{n}} \bigg|_p = \frac{1}{V_p} \sum_{l=1}^{M} \sum_{m} \left( \nabla \xi^l_{m} \cdot \hat{n} \right) \hat{m}_l \int_{\Omega^l_{\hat{n}}} \xi^l_{(p)} dS.
\]

(3.29)

The quantity \( \nabla \xi^l_{m} \cdot \hat{n} \) has been taken out of the integral, since \( \nabla \xi^l_{m} \) is constant. It can be shown that [Peterson et al., 1998]

\[
\int_{\Omega^l_{\hat{n}}} \xi^l_{q} dS = \frac{S^l_{\hat{n}}}{3},
\]

(3.30)

where \( S^l_{\hat{n}} \) is the surface area of domain \( \Omega^l_{\hat{n}} \). Defining

\[
S_p = \frac{1}{3} \sum_{t} S^t,
\]

(3.31)

where \( t \) runs over all \( T_{p,\hat{n}} \) triangles sharing node \( p \) and belonging to the bounding surface, with \( S^t \) denoting the triangle area, we can rewrite equation (3.29) as

\[
\frac{1}{t_p} \frac{\partial \hat{m}}{\partial \hat{n}} \bigg|_p = \frac{S_p}{V_p} \sum_{l=1}^{M} \sum_{m} \left( \nabla \xi^l_{m} \cdot \hat{n} \right) \hat{m}_l.
\]

(3.32)

It is easily recognized that the double summation in (3.32) is simply the finite element representation of \( \partial \hat{m} / \partial \hat{n} = \nabla \hat{m} \cdot \hat{n} \), when \( \hat{m} \) is expanded in terms of linear basis functions.
Figure 3.5: Indirect exchange between two magnetic moments separated by a non-magnetic spacer (interlayer) in the (a) continuum and (b) finite element model. In (a) the two considered magnetic moments belong to the infinitesimal volumes $\delta V_+$ and $\delta V_-$, while in (b) the corresponding moments belong to effective volumes associated with node $p$ and $q$ as expressed in (3.10).

Consequently, (3.32) can hold only if the depth $t_p$ associated with boundary node $p$ equals the ratio of the effective volume to the effective surface belonging to the same node and lying on the body boundary $S$, i.e.,

$$t_p = \frac{V_p}{S_p}.$$  \hspace{1cm} (3.33)

This could have been anticipated from the transcription $\delta t = \delta V / \delta S \rightarrow t_p$ of (2.52).

### 3.2.2 Interlayer Exchange Field

When two bodies are indirectly exchange coupled (across an interlayer) with interfacial exchange energy density $J$ (erg/cm$^2$), the resulting exchange field on the magnetic moment $\delta \mu_+ = M_s \delta V_+ \hat{m}_+ \delta V_+$, contained within volume $\delta V_+$ situated at the interface opposite of moment $\delta \mu_-$ (Fig. 3.5a), has the form (2.57), i.e.,

$$H_{\text{ex},\delta V_+} = -\frac{1}{M_s \delta V_+} \frac{\delta E_{\text{ex}}}{\delta \hat{m}_+ \delta V_+} = \frac{J_{\delta S_+}}{M_s \delta V_+} \delta t_+ \hat{m}_\delta V_-.$$  \hspace{1cm} (3.34)

Assuming a mesh where the two coupled surfaces are identically triangulated so as to form triangle pairs (Fig. 3.5b), the interlayer exchange field at interface node $p$ can be
Figure 3.6: (a) When node $p$ is an edge node situated at the exchange coupling interface across from node $q$, only interfacial triangles (shaded violet) sharing node $p$ enter the sum in (3.38). (b) For the case that node $p$ is indirectly exchange coupled across more than one interface, the effective depth $t_{pq}$ appearing in (3.39) is calculated per interface according to (3.37). For an interface containing node pair $(p, q)$, only triangles belonging to that particular interface contribute to $t_{pq}$ via $S_{pq}$, as indicated by the color correspondence between the triangle outlines and respective indirectly exchange coupled bodies.

Transcribed from (3.34) to the finite element form

$$H^\text{ex}_p = \frac{J_{pq}}{M_{s,p} t_{pq}} \hat{m}_q,$$

(3.35)

where $\hat{m}_q$ is the unit magnetization vector coefficient associated with node $q$ which is opposite to node $p$ across the interface. Since different triangle pairs may be coupled with different energy densities, $J_{pq}$ is obtained as the weighted average over all $T_{pq}$ interface triangle pairs having $(p, q)$ for a common node pair,

$$J_{pq} = \frac{\sum_{t}^T J^t S^t}{\sum_{t}^T S^t}.$$

(3.36)

Here, $J^t$ denotes the exchange coupling energy density per triangle pair whose interface area is $S^t$. The effective depth in (3.35) is given by (cf. (3.33))

$$t_{pq} = \frac{V_p}{S_{pq}},$$

(3.37)

where $V_p$ is the volume associated with node $p$, as given in (3.10), and

$$S_{pq} = \frac{1}{3} \sum_{t}^T S^t.$$

(3.38)
The sum in (3.38) is over the triangles of $p$ belonging to the exchange coupling interface, and not over all $T_{p,n}$ boundary triangles sharing node $p$, as was the case in (3.31). The distinction is important for the case of edge or corner nodes. For edge node $p$ in Fig. 3.6a, only three of its six boundary triangles belong to the exchange coupling interface, hence the sum in the above expression for $S_{pq}$ should be taken over only these three triangles. When an edge node $p$ is indirectly exchange coupled across more than one exchange coupling interface, as illustrated in Fig. 3.6b, the interlayer exchange field at node $p$ is computed according to the generalized expression

$$H_{p}^{\text{ex}} = \sum_{q \in (p,q)} \frac{J_{pq}}{M_{s,p} \mu_{pq}} \hat{m}_{q},$$

(3.39)

where the sum is over all nodes $q$ that form interfacial node pairs with $p$.

Equation (3.39) is commonly used for the computation of the interlayer exchange field in micromagnetic solvers based on the linear basis finite element representation. However, deriving $H_{p}^{\text{ex}}$ from the variation of the associated energy functional in discretized form yields a different expression, one we argue is in greater conformity to the finite element linear basis formalism. The interlayer exchange energy functional in continuum form (section 2.1.7) reads

$$E_{\text{ex}} = -\int_{S} J(r) \hat{m}_{+}(r) \cdot \hat{m}_{-}(r) dS. \quad (3.40)$$

This can be written in discretized form as

$$E_{\text{ex}} = -\sum_{t=1}^{T_{\text{int}}} J_{t}^{\text{int}} \int_{S_{t}} \left( \sum_{k=1}^{3} \hat{m}_{k}^{t+} \zeta_{k}^{t+} \right) \cdot \left( \sum_{k=1}^{3} \hat{m}_{k}^{t-} \zeta_{k}^{t-} \right) dS. \quad (3.41)$$

The integration in (3.41) over the exchange coupling interface(s) has been broken up into integration over all $T_{\text{int}}$ interfacial triangle pairs. Since only the nodal magnetization unit vectors associated with vertices of these triangles contribute to the expansion of the magnetization at the exchange coupling interface(s), we have chosen to use linear basis functions $\zeta_{k}^{t}$ associated with triangles $t$ and triangle vertices $k$, rather than the linear basis functions $\xi_{k}^{l}$ associated with tetrahedra and tetrahedral vertices. The interlayer exchange field at node $p$ is obtained from the first order variation of the discretized energy with respect to $\hat{m}_{p}$,

$$H_{p}^{\text{ex}} = -\frac{1}{M_{s,p} V_{p}} \frac{\partial E_{\text{ex}}}{\partial \hat{m}_{p}} = \frac{1}{M_{s,p} V_{p}} \sum_{t=1}^{T_{\text{int}}} J_{t}^{\text{int}} \int_{S_{t}} \zeta_{(p)}^{t+} \left( \sum_{k=1}^{3} \hat{m}_{k}^{t-} \zeta_{k}^{t-} \right) dS. \quad (3.42)$$
A global index representing a node on the (+) side of an interface is denoted by \( p \), while \( k \) is a local index representing one of the nodes of a given triangle \( t_- \) residing on the opposite (−) side. Equation (3.42) can be rewritten as

\[
H_{\text{ex}}^p = \frac{1}{M_{s,p} \Delta V_p} \sum_{t=1}^{T_{\text{int}}} J^t \sum_{k=1}^{3} \hat{m}_k^t \int_{S_t} \zeta_{(p)}^t \zeta_k^t dS.
\]

Using the identity \( \int_{S} \zeta_1^m \zeta_2^n \zeta_3^p dS = \frac{2m!n!p!}{(2+m+n+p)!} S \) [Peterson et al., 1998], where \( \zeta_1, \zeta_2, \zeta_3 \) are the linear basis functions associated with the three nodes of a single triangle of area \( S \), and \( m, n, p \) are exponents, we have

\[
H_{\text{ex}}^p = \frac{1}{M_{s,p} \Delta V_p} \sum_{t=1}^{T_{\text{int}}} J^t S_t \sum_{k=1}^{3} (1 + \delta_{(p)k}) \hat{m}_k^t.
\]

Here, \( \delta_{(p)k} \) equals unity if global node \( p \) coincides with vertex \( k \) of triangle \( t_- \), otherwise it equals zero. When the mesh size is sufficiently smaller than the exchange length, the interlayer exchange field in (3.44) can be reduced to

\[
H_{\text{ex}}^p = \frac{1}{M_{s,p} \Delta V_p} \sum_{q \in (p,q)} \langle J \rangle_{pq} \hat{m}_q^t, \quad \text{where} \quad q \text{ is a node opposite to node } p \text{ across an exchange coupling interface},
\]

\( \langle J \rangle_{pq} \) is the averaged interfacial exchange energy density associated with node pair \( (p,q) \), and \( t_{pq} = V_p S_{pq} \), with \( S_{pq} = \sum_{t} \int_{S_t} \zeta_{(p)k}^t dS = \frac{1}{3} \sum_{t} S_t^t \). The reduced expression is equivalent to (3.39). The difference between (3.39) and (3.44) is that the latter expression accounts for the across-the-interface mixing of the linear basis functions expanding the magnetization at opposite sides of the exchange coupling interface(s), while the former expression ignores this mixing contribution. Both expressions should yield nearly identical fields when the mesh size is well below the characteristic length scales associated with the problem.

### 3.2.3 Bulk and Surface Anisotropy Fields

The bulk and surface (or interface) anisotropy fields for the uniaxial case, derived in sections 2.2.4 and 2.2.5, are

\[
H_{\text{anis,}\delta V} = -\frac{1}{M_{s,\delta V} \delta V} \frac{\delta E_{\text{anis}}}{\delta \hat{m}_{\delta V}} = \frac{2K_{4V}}{M_{s,\delta V}} \left( \hat{m}_{\delta V} \cdot \hat{k}_{\delta V} \right) \hat{k}_{\delta V},
\]

\[
H_{\text{anis},\delta V} = -\frac{1}{M_{s,\delta V} \delta V} \frac{\delta E_{\text{anis}}}{\delta \hat{m}_{\delta V}} = \frac{2K_{4V}^s}{M_{s,\delta V} \delta t} \left( \hat{m}_{\delta V} \cdot \hat{k}_{\delta V}^s \right) \hat{k}_{\delta V}^s.
\]

In the finite element representation, this straightforwardly transcribes to

\[
H_{\text{anis}}^p = \frac{2K_p}{M_{s,p}} \left( \hat{m}_p \cdot \hat{k}_p \right) \hat{k}_p,
\]

(3.47)
\[ H_{p}^{\text{anis},s} = \sum_{i \in (p/i)} \frac{2K_{p/i}^{s}}{M_{s,p}^{p/i}} \left( \hat{m}_{p} \cdot \hat{k}_{p/i}^{s} \right) \hat{k}_{p/i}^{s}. \]  

where the sum in (3.48) runs over all surfaces \( i \) supporting surface anisotropy and containing node \( p \). The effective bulk anisotropy energy density \( K_{p} \) and easy axis direction \( \hat{k}_{p} \) associated with node \( p \) are computed by weighted averaging over surrounding tetrahedra as done for saturation magnetization and exchange stiffness in (3.8) and (3.9). The effective surface anisotropy energy density \( K_{p/i}^{s} \) and easy axis direction \( \hat{k}_{p/i}^{s} \) associated with boundary node \( p \) and surface \( i \) are obtained through weighted averaging over all \( T_{p/i} \) triangles sharing node \( p \) and belonging to surface \( i \),

\[ K_{p/i}^{s} = \frac{T_{p/i}}{T_{l} S_{t}} \sum_{t} K_{s,t} S_{t}, \]

\[ \hat{k}_{p/i}^{s} = \frac{T_{p/i}}{T_{l} S_{t}} \sum_{t} \hat{k}_{s,t} S_{t}. \]

The effective depth \( t_{p/i} \) in (3.48) associated with node \( p \) and surface \( i \) is computed as \( t_{p/i} = V_{p}/S_{p/i} \), where \( S_{p/i} = \frac{1}{3} \sum_{t} S_{t} \), with the sum running over all triangles of \( p \) belonging to surface \( i \), analogously to (3.38), and not over all boundary triangles of node \( p \), as in (3.31). The distinction is important for the case of edge or corner nodes, as discussed in section 3.2.2.

More rigorously, the bulk and surface anisotropy fields at the nodes can be derived from the variation of the corresponding energy functionals cast in discretized form. Using previously described linear basis functions \( \xi_{k}^{l}(r) \) to represent \( \hat{m}(r) \), the discretized bulk anisotropy energy is obtained from (2.16),

\[ E_{\text{anis}}^{\text{dis}} = -\sum_{l=1}^{M} K^{l} \int_{V} \left[ \sum_{k=1}^{4} \xi_{k}^{l} \hat{m}_{k}^{l} \right]^{2} dV, \]

with \( l \) running over all \( M \) tetrahedrons of the model, and \( k \) running over the four vertices of each tetrahedron \( l \). The bulk anisotropy field at node \( p \) is now derived as

\[ H_{p}^{\text{anis}} = -\frac{1}{M_{s,p} V_{p}} \sum_{l=1}^{M} K^{l} \int_{V} \xi_{(p)}^{l} dV. \]

Using identity (3.11), this gives

\[ H_{p}^{\text{anis}} = \frac{2}{M_{s,p} V_{p}} \hat{m}_{p} \cdot \sum_{l}^{M} \frac{K^{l} V^{l}}{4} \hat{k}^{l} \hat{k}^{l}, \]
with $l$ now running over all $M_p$ tetrahedrons having node $p$ for a common vertex. In the above equation, $\hat{k}^l \hat{k}^l$ is a dyadic product

$$\hat{k}^l \hat{k}^l = \begin{pmatrix} k^l_{lx} k^l_{lx} & k^l_{lx} k^l_{ly} & k^l_{lx} k^l_{lz} \\ k^l_{ly} k^l_{lx} & k^l_{ly} k^l_{ly} & k^l_{ly} k^l_{lz} \\ k^l_{lz} k^l_{lx} & k^l_{lz} k^l_{ly} & k^l_{lz} k^l_{lz} \end{pmatrix}.$$  

(3.54)

Formulating the anisotropy field in terms of an inner product between the magnetization unit vector $\hat{m}_p$ and the dyadic tensor $\sum_{l} K^l V^l \hat{k}^l \hat{k}^l$, as done in (3.53), avoids the inclusion of $\hat{m}_p$ in the sum. The benefit is that the summation $\sum_{l} K^l V^l \hat{k}^l \hat{k}^l$ need now be performed only once, as the resulting tensor may be reused at each simulation time step, thus eliminating unnecessary reevaluations.

Finally, for the surface anisotropy field at node $p$, similarly to (3.53), we have

$$H_{p}^{\text{anis}, s} = \frac{2}{M_{s,p} V_p} \hat{m}_p \sum_{t} \frac{K^{s,t} S^{t}}{3} \hat{k}^{s,t} \hat{k}^{s,t},$$  

(3.55)

where $t$ runs over all $T_p$ surface triangles sharing node $p$.

Though expressions (3.47) and (3.48) are not equivalent with expressions (3.53) and (3.55), both should give near-equal values for the respective fields when mesh dimensions are sufficiently below the critical lengths characterizing magnetization texture.

### 3.2.4 Magnetostatic Field

Equation (2.64) can be directly transcribed to the finite element form, writing the magnetostatic field at node $p$ as

$$H_p^{\text{ms}} = -\nabla \sum_{l=1}^{M} \int_{\Gamma_l} \frac{\nabla' \cdot \left( M_s(r') \sum_{k=1}^{4} \zeta^l_k(r') \hat{m}^l_k \right)}{|r' - r_p|} dV'$$

$$-\nabla \sum_{t=1}^{T_{\hat{h}}} \int_{\Omega_{\hat{h}}} \frac{\hat{n}' \cdot \left( M_s(r') \sum_{k=1}^{3} \zeta^s_k(r') \hat{m}^s_k \right)}{|r' - r_p|} dS'.$$  

(3.56)

Here, $l$ runs over all $M$ tetrahedrons, $t$ runs over all $T_{\hat{h}}$ tetrahedral faces belonging to bounding surfaces, and $M_s$ is assumed constant within each tetrahedron. The coordinate of node $p$ is given by $r_p$. Equation (3.56) can conveniently be written as

$$H_p^{\text{ms}} = -\nabla \sum_{l=1}^{M} \int_{\Gamma_l} \frac{p_l}{|r' - r_p|} dV' - \nabla \sum_{t=1}^{T_{\hat{h}}} \int_{\Omega_{\hat{h}}} \frac{\sigma_t}{|r' - r_p|} dS',$$  

(3.57)
where
\[ \rho_l = -\nabla' \cdot \left( M_s(r') \sum_{k=1}^{4} \xi_k(r') \hat{m}_k \right), \tag{3.58} \]
\[ \sigma_t = M_s(r') \hat{n}' \cdot \sum_{k=1}^{3} \zeta_k(r') \hat{m}_k \tag{3.59} \]
are the effective magnetic volume and surface charges corresponding to tetrahedron \( l \) and boundary tetrahedral face \( t \), respectively. It can be seen that \( \rho_l \) is constant within each tetrahedron \( l \), while \( \sigma_t \) is a linear function of space. The direct evaluation of the magnetostatic field at all \( N \) mesh nodes requires \( O(N^2) \) operations, which presents a major computational chokepoint for large-scale simulations of magnetization dynamics. Efficient computational techniques used to overcome this problem are summarized in section 8.1. Quadrature rules and analytical integration used for singularity extraction are discussed in [Chang et al., 2011].

### 3.2.5 Zeeman Field

Assuming the external field does not vary significantly over distances comparable to the tetrahedral dimensions, as should be the case for properly discretized models, the transcription of the Zeeman field from the continuum approach to the finite element representation \( H_{\text{Zee},SV} \rightarrow H_{\text{Zee},p} \) leads to
\[ H_{\text{Zee},p} = H_{\text{Zee}}(r_p) = H_a(r_p), \tag{3.60} \]
where \( r_p \) is the system coordinate vector pointing to node \( p \), and \( H_a(r) \) is the externally applied field.

**Acknowledgements:** Chapter 3, in part, is based on the journal article: R. Chang, S. Li, M. V. Lubarda, B. Livshitz, V. Lomakin, “FastMag: Fast micromagnetic solver for large-scale simulations,” *Journal of Applied Physics* 109, 07D358 (2011). The dissertation author was the contributing author to this article.
4 Finite Element Modeling of Spin Transfer Torques

The finite element linear basis representation from chapter 3 is used to model spin transfer torques in patterned multilayer spin valves and in extended magnetic systems. In-plane and out-of-plane spin transfer torques are discussed in the context of spin valves and magnetic tunnel junctions in current-perpendicular-to-plane geometry. Field-like expressions for the two torques are derived. The adiabatic and nonadiabatic contributions to spin transfer torques are discussed in the context of magnetically continuous systems. The modeling of Oersted fields in conjunction with spin transfer torques is presented.

4.1 Spin Transfer Torques in Multilayer Spin Valves with Current-Perpendicular-to-Plane Geometry

4.1.1 All-Metallic Spin Valves

Assuming full absorption of the transverse component of the spin current at the normal metal/ferromagnet (NM/FM) interfaces (section 2.1.8), neglecting spin pumping, and ignoring coupling to the orbital angular momentum, the spin transfer torque (STT) on either magnetic layer of a FM/NM/FM multilayer stack with current flowing perpendicular to the plane, can, to a reasonable approximation, be expressed as

\[ \tau_{\text{STT},+} = \eta(\theta) \frac{1}{2} \frac{\hbar}{2e} \hat{m}_+ \times \hat{m}_+ \times \hat{m}_-. \] (4.1)

Above, \( \hat{m}_+ \) and \( \hat{m}_- \) denote the unit magnetization vectors of the two magnetic layers in the stack (subscripts + and − are arbitrary and interchangeable). The angular dependence of the STT efficiency is specified by

\[ \eta(\theta) = \frac{q_p}{A + B \cos \theta} + \frac{q_n}{A - B \cos \theta}, \] (4.2)
Figure 4.1: (a) Finite element model of a spin valve nanopillar composed of two magnetic layers separated by a nonmagnetic normal metal spacer layer (spacer layer not shown). (b) Zoom-in showing a pairwise correspondence between interface nodes.

where \( q_p, q_n, A, \) and \( B \) are device dependent constants [Xiao et al., 2005], and \( \cos \theta = \hat{m}_i \cdot \hat{m}_j \). The remaining symbols in equation (4.1) are the reduced Planck constant \( \hbar \), electric current density \( J \), the elementary charge \( e \), and the effective depth \( \delta t \) across the interface into the magnetic layer over which the spin transfer torque is distributed. Assuming that spin transfer is purely an interface effect, the effective depth can be taken as infinitesimal, i.e., \( \delta t \to 0 \). We now turn to the modeling of spin transfer torque within the linear basis finite element framework described in chapter 3.

Figure 4.1a shows a cylindrical spin valve nanopillar composed of two magnetic layers separated by a nonmagnetic normal metal spacer layer (spacer layer not shown). Figure 4.1b shows the mesh that defines the discretized model in more detail. A tetrahedral discretization scheme is chosen that yields identical triangulation of the two NM/FM interfaces. The identical triangulation implies a pairwise correspondence between mesh nodes on opposite sides of the spacer layer. The spin torque acting on the magnetic moment in the vicinity of node \( i \) (Fig. 4.1b) can be represented in the finite element representation as

\[
\tau^{\text{STT}}_i = \zeta_i \eta(\theta_{ij}) \frac{1}{t_i} \frac{\hbar}{2} \frac{J_{ij}}{e} \hat{m}_i \times \hat{m}_i \times \hat{m}_j,
\]

(4.3)

where \( \hat{m}_i \) is the unit magnetization vector of node \( i \), \( \hat{m}_j \) is the unit magnetization vector of node \( j \) which is directly opposite of node \( i \) across the spacer layer, \( \cos \theta_{ij} = \hat{m}_i \cdot \hat{m}_j \), \( t_i \) is the effective depth associated with node \( i \) and depends on the local mesh dimensions, and \( \zeta_i \) is an indicator function which equals unity if node \( i \) belongs to a NM/FM interface, and is zero otherwise. The explicit expression for \( t_i \) can be found in equation (2.33). This equation gives the prescription of how and infinitesimal quantity \( \delta t \to 0 \) takes on a finite
value in the linear basis finite element representation based on tetrahedral discretization.

If the total electric current $I_{\text{tot}}$ flowing through the spin valve is externally controlled, the current density $J_i$ in equation (4.3) can be approximated by $J_i = I_{\text{tot}}/S$, where $S$ is the spin valve cross-sectional area. However, this approximation fails when domain walls or highly nonuniform magnetization states develop in one or both of the magnetic layers (Fig. 4.2a). In this case, the current density needs to be redistributed to account for the giant magnetoresistance (GMR) effect (section 12.1.1). GMR can be modeled by associating to each interfacial node pair $(i, j)$ a conductivity channel whose channel specific resistance is given by $\rho_{ij} = 1 + r_{\text{MR}}(1 - \cos \theta_{ij})/2$. Here, $r_{\text{MR}} = (R_{\text{AP}} - R_{\text{P}})/R_{\text{P}}$ is the GMR ratio, $R_{\text{P}}$ and $R_{\text{AP}}$ are the resistances for the parallel and antiparallel configurations, and $\cos \theta_{ij} = \hat{m}_i \cdot \hat{m}_j$, as before. The spin valve channel model is schematically represented in Fig. 4.2b. The current density within each channel can now be expressed as

$$J_{ij} = \sigma_{ij} V,$$  \hspace{1cm} (4.4)

where $\sigma_{ij} = 1/\rho_{ij}$ is the channel specific conductance, and $V$ is the instantaneous voltage difference between the two NM/FM interfaces. The current through each channel may be written as

$$I_{ij} = G_{ij} V,$$  \hspace{1cm} (4.5)

where $G_{ij} = \sigma_{ij} S_{ij}$ is the conductance, and $S_{ij}$ the channel cross-sectional area, or correspondingly, the effective surface area associated with node $i$ (or $j$, owing to the identical triangulation of interfaces; Fig. 4.1). The expression for $S_{ij}$ is given in (3.31). The voltage in equation (4.4) or (4.5) can be obtained from the conservation of charge flow $I_{\text{tot}} = \sum_{(i,j)} I_{ij}$ as

$$V = I_{\text{tot}}/G,$$  \hspace{1cm} (4.6)

where

$$G = \sum_{(i,j)} G_{ij} \hspace{1cm} (4.7)$$

represents the total conductivity of the assemblage of parallel channels going through the spacer layer. The calculated current redistribution due to magnetoresistance for the magnetization configuration illustrated in Fig. 4.2a is shown in Fig. 4.2c.

Equations (4.4)–(4.7) remain reasonably valid for the more general case involving a stack of an arbitrary number of layers (Fig. 4.3), as long as the constituent layers are not critically thin [Thiaville et al., 2005]. Equation (4.6) is then used to calculate the
Figure 4.2: (a) Spin valve of Fig. 4.1 with magnetization shown. Bottom (fixed) layer is uniformly magnetized upwards, while the top (free) layer has a nonuniform magnetization containing a vortex. (b) Conducting channels of variable resistivity used for modeling magnetoresistance to account for current redistribution. (c) Computed current density at free layer interface for the magnetization configuration illustrated in (a). The current density is the greatest where the free layer magnetization is parallel to that of the fixed layer, i.e., at the vortex core.
Figure 4.3: A spin valve model consisting of an arbitrary number of layers.

voltage drop across each spacer layer in the multilayer spin valve. The conductance $G$ in equation (4.7) for each spacer is obtained as a sum over only the channels belonging to that spacer, and not over all channels across all spacers.

In many cases it is desired that the voltage across the device be controlled instead of the current. If the total voltage $V_{tot}$ across the device is known, the voltage drop over each resistor in Fig. 4.3 can be found, and $I_{ij}$ can be again obtained from equation (4.5). The current density at interfacial node $i$ and corresponding opposite node $j$ ($J_i = J_j = J_{ij}$) can now be expressed as

$$J_{ij} = \frac{I_{ij}}{S_{ij}}. \quad (4.8)$$

Having expressed all quantities in (4.3), we can now add the STT term to the Landau-Lifshitz-Gilbert (LLG) equation to describe the magnetization dynamics of a spin valve multilayer stack under the influence of spin polarized currents and magnetic fields,

$$\frac{d\hat{m}_i}{dt} = -\gamma \hat{m}_i \times \mathbf{H}^{eff}_i + \alpha_i \hat{m}_i \times \frac{d\hat{m}_i}{dt} + \zeta_i \eta(\theta_{ij}) \frac{1}{t_i} \frac{\hbar}{2} \frac{J_i}{e} \hat{m}_i \times \hat{m}_i \times \hat{m}_j. \quad (4.9)$$

This can be rewritten as

$$\frac{d\hat{m}_i}{dt} = -\gamma \hat{m}_i \times \left( \mathbf{H}^{eff}_i + \mathbf{H}^{STT}_i \right) + \alpha_i \hat{m}_i \times \frac{d\hat{m}_i}{dt}, \quad (4.10)$$

where

$$\mathbf{H}^{STT}_i = -\zeta_i \frac{1}{\gamma} \eta(\theta_{ij}) \frac{1}{t_i} \frac{\hbar}{2} \frac{J_i}{e} \hat{m}_i \times \hat{m}_j. \quad (4.11)$$
is a convenient field-like expression for the STT term, which can simply be added to the effective field $H_{i}^{\text{eff}}$. We note, however, that $H_{i}^{\text{eff}}$ is fundamentally different from $H_{i}^{\text{STT}}$. The former can be derived from the variation of the micromagnetic free energy (section 2.2), while the latter is akin to the damping term, which does not preserve time reversal symmetry, and hence implies energy dissipation/pumping.

Equation (4.10) can be transformed, following the later transformation from equation (4.19) to (4.21), to an explicit form

$$\frac{d\hat{m}_i}{dt} = -\frac{\gamma}{1 + \alpha_i^2} \left[ \hat{m}_i \times \left( H_{i}^{\text{eff}} + H_{i}^{\text{STT}} \right) + \alpha_i \hat{m}_i \times \hat{m}_i \times \left( H_{i}^{\text{eff}} + H_{i}^{\text{STT}} \right) \right].$$

(4.12)

It has been shown that the appearance of $H_{i}^{\text{STT}}$ in the second term on the right-hand side (4.12) does not noticeably influence magnetization dynamics in spin valve structures and can be omitted. It has been argued in fact that it is more appropriate to add the STT term $\tau_{i}^{\text{STT}}$ to the Gilbert form (2.2) rather than to the Landau-Lifshitz equation (2.3) [Xiao et al., 2005]. In this case $H_{i}^{\text{STT}}$ never appears in the second term of equation (4.12).

### 4.1.2 Magnetic Tunnel Junctions

While in all-metallic spin valves the transverse component of the incident spin current is rather fully absorbed at the NM/FM interface, in metallic tunnel junctions (MTJs) an appreciable fraction of the transverse spin component may yet be transmitted into the receiving ferromagnet owing to the inherently more selective tunneling process (section 2.1.8). Accordingly, micromagnetic modeling of spin transfer torques in MTJs involves the so-called out-of-plane torque contribution in addition to the in-plane torque contribution (section 2.1.8). The out-of-plane torque is given by

$$\tau_{\text{OP STT},+}^{\text{STT}} = \beta \eta(\theta) \frac{1}{\delta t} \frac{\hbar}{2} \frac{J}{e} \hat{m}_+ \times \hat{m}_-. $$

(4.13)

All symbols in the above expression have the same meaning as in equation (4.1), $\beta$ being the only new parameter denoting the relative magnitude of the out-of-plane torque $\tau_{\text{OP STT},+}$ with respect to the in-plane torque contribution expressed in (4.1). The out-of-plane contribution is added along with the in-plane STT contribution to the LLG equation, and expressed in the finite element representation as

$$\frac{d\hat{m}_i}{dt} = -\gamma \hat{m}_i \times H_{i}^{\text{eff}} + \alpha_i \hat{m}_i \times \frac{d\hat{m}_i}{dt} + \zeta_i \eta(\theta_{ij}) \frac{1}{\delta t} \frac{\hbar}{2} \frac{J_i}{e} \hat{m}_i \times \hat{m}_i \times \hat{m}_j$$

$$+ \beta \zeta_i \eta(\theta_{ij}) \frac{1}{\delta t} \frac{\hbar}{2} \frac{J_i}{e} \hat{m}_i \times \hat{m}_j. $$

(4.14)
In explicit (Landau-Lifshitz) form, this reads
\[
\frac{d\hat{m}_i}{dt} = -\frac{\gamma}{1 + \alpha_i} \left[ \hat{m}_i \times \left( H_i^{\text{eff}} + H_i^{\text{STT}} \right) + \alpha_i \hat{m}_i \times \hat{m}_i \times \left( H_i^{\text{eff}} + H_i^{\text{STT}} \right) \right]. \tag{4.15}
\]
Here,
\[
H_i^{\text{STT}} = H_i^{\text{IP STT}} + H_i^{\text{OP STT}}, \tag{4.16}
\]
with the field quantity
\[
H_i^{\text{IP STT}} = -\zeta_i \gamma \eta(\theta_{ij}) \frac{\hbar}{2} J_i \frac{e}{\hbar} \hat{m}_i \times \hat{m}_j \tag{4.17}
\]
accounting for the in-plane spin transfer torque \(\tau_{\text{IP,STT}}\) given by (4.1), and
\[
H_i^{\text{OP STT}} = -\zeta_i \gamma \beta \eta(\theta_{ij}) \frac{\hbar}{2} J_i \frac{e}{\hbar} \hat{m}_j \tag{4.18}
\]
accounting for the out-of-plane STT contribution (4.13), which results from the incomplete absorption of the transverse component of spin current at the NM/FM interface.

Related to the differences in band structure between tunnel junctions and all-metallic spin valves, besides the dissimilarity in absorption of the transverse spin component, is the difference of the respective forms of \(\eta(\theta)\), which, for the case of tunnel barriers, shows reduced dependence on \(\theta\), and is often modeled flat, i.e., \(\eta(\theta) = \eta_0\) (section 12.2). A discussion of \(\eta(\theta)\) and its effect on the operation of spin valve devices is given in section 12.1.4.

### 4.2 Spin Transfer Torques in Magnetically Continuous Systems

In magnetically continuous textured systems the effect of spin polarized currents on the magnetization may be expressed in implicit form [Zhang and Li, 2004, Thiaville et al., 2005] as
\[
\frac{d\hat{m}}{dt} = -\gamma \hat{m} \times H_{\text{eff}} + \alpha \hat{m} \times \frac{d\hat{m}}{dt} - (u \cdot \nabla \hat{m}) + \beta \hat{m} \times (u \cdot \nabla \hat{m}) \tag{4.19}
\]
The first term on the right-hand side represents the precession of the magnetization around the micromagnetic effective field \(H_{\text{eff}}\). The second term represents the damping torque in Gilbert form. The left-hand side together with the first two terms on the right comprises the LLG equation, to which now added are the adiabatic and nonadiabatic spin transfer torque (STT) contributions (section 2.1.8), where
\[
u = \frac{1}{M_s} \frac{g\hbar}{4m_e} PJ = \frac{1}{M_s} \frac{g\mu_B}{2e} PJ \tag{4.20}
\]
is the velocity vector directly proportional to the current density $J$, and modulated by the spin current polarization $P$ and background moment density $M_\text{s}$. In (4.20), $g$ is the g-factor of an electron, $\hbar$ is the reduced Planck’s constant, while $m_e$ and $e$ are the electron mass and absolute charge, respectively. The quantity $\nabla \hat{m}$, appearing in both STT terms, represents the dyadic product of the gradient vector operator and the magnetization unit vector. An alternative but equivalent means to express $u \cdot \nabla \hat{m}$ is to write $(u \cdot \nabla) \hat{m}$.

Finally, $\beta$ in the second STT term is the nonadiabaticity factor defining the strength of the nonadiabatic contribution.

It is favorable to rework equation (4.19) into an explicit form, which will be more amenable to a number of numerical integration routines. Replacing $d\hat{m}/dt$ on the right-hand side of equation (4.19) with the expression for $d\hat{m}/dt$ as given by the right-hand side itself, and expanding, one obtains

$$
\frac{d\hat{m}}{dt} = -\gamma \hat{m} \times H_{\text{eff}} - \alpha \gamma \hat{m} \times \hat{m} \times H_{\text{eff}} + \alpha^2 \hat{m} \times \hat{m} \times \frac{d\hat{m}}{dt} - \alpha \hat{m} \times (u \cdot \nabla \hat{m}) \\
+ \alpha \beta \hat{m} \times \hat{m} \times (u \cdot \nabla \hat{m}) - (u \cdot \nabla \hat{m}) + \beta \hat{m} \times (u \cdot \nabla \hat{m}).
$$

(4.21)

The third term on the right-hand side, by virtue of vector identity $a \times b \times c = b (a \cdot c) - c (a \cdot b)$, can be rewritten as $\hat{m} \times \hat{m} \times \frac{d\hat{m}}{dt} = \hat{m} \left( \hat{m} \cdot \frac{d\hat{m}}{dt} \right) - \frac{d\hat{m}}{dt} (\hat{m} \cdot \hat{m})$, thus simplifying to $-\frac{d\hat{m}}{dt}$, as $\hat{m} \cdot \frac{d\hat{m}}{dt} = 0$, owing to the constraint $|\hat{m}| = 1$ and its implication $\frac{d\hat{m}}{dt} \perp \hat{m}$.

Consequently,

$$
\frac{d\hat{m}}{dt} = -\frac{1}{1 + \alpha^2} \left[ \gamma \hat{m} \times H_{\text{eff}} + \gamma \alpha \hat{m} \times \hat{m} \times H_{\text{eff}} + \alpha \hat{m} \times (u \cdot \nabla \hat{m}) \\
- \alpha \beta \hat{m} \times \hat{m} \times (u \cdot \nabla \hat{m}) + u \cdot \nabla \hat{m} - \beta \hat{m} \times (u \cdot \nabla \hat{m}) \right].
$$

(4.22)

The nonadiabatic contribution to the spin transfer torque can be expressed in field-like form, to yield

$$
\frac{d\hat{m}}{dt} = -\frac{\gamma}{1 + \alpha^2} \left[ \hat{m} \times \left( H_{\text{eff}} + H_{\text{STT}}^{\text{nonadia}} \right) + \alpha \hat{m} \times \hat{m} \times \left( H_{\text{eff}} + H_{\text{STT}}^{\text{nonadia}} \right) \right] + \tau_{\text{STT}}^{\text{adia}},
$$

(4.23)

where

$$
\tau_{\text{STT}}^{\text{adia}} = -\frac{\alpha}{1 + \alpha^2} \hat{m} \times (u \cdot \nabla \hat{m}) - \frac{1}{1 + \alpha^2} u \cdot \nabla \hat{m},
$$

(4.24)

and

$$
H_{\text{STT}}^{\text{nonadia}} = -\frac{\beta}{\gamma} u \cdot \nabla \hat{m}.
$$

(4.25)

Equation (4.23) is the final form of the explicit equation governing magnetization dynamics in magnetically continuous systems under the influence of spin polarized currents whose
contribution to the torque is reflected in the adiabatic and nonadiabatic terms. The fact that the nonadiabatic contribution to the spin transfer torque could be cast as an effective field of the form (4.25) is consistent with the physical understanding of its effect as discussed in [Thiaville et al., 2005].

Having expressed equation (4.19) in explicit form (4.23), we can recast equation (4.23) in the finite element linear basis representation. We assume the system has been discretized by tetrahedrons as discussed in chapter 3. The main quantity which appears in both the adiabatic and nonadiabatic term in equation (4.23) is \( \varsigma = \mathbf{u} \cdot \nabla \hat{\mathbf{m}} \). In the finite element representation, \( \varsigma \) at node \( p \) takes the form

\[
\varsigma_{\mid p} = (\mathbf{u} \cdot \nabla \hat{\mathbf{m}})_{\mid p} \quad \rightarrow \quad \varsigma_{p} = \mathbf{u}_{p} \cdot \sum_{l} \sum_{k=1}^{M_{p}} \nabla \xi_{l}^{k} \hat{\mathbf{m}}_{k}^{l} = \sum_{l} \sum_{k=1}^{M_{p}} \mathbf{u}_{p} \cdot \nabla \xi_{l}^{k} \hat{\mathbf{m}}_{k}^{l},
\]

where \( l \) runs over all \( M_{p} \) tetrahedra having node \( p \) for a common vertex, and \( k \) runs over the four vertices of each tetrahedron in the sum. The expression \( \nabla \xi_{l}^{k} \) takes on the familiar form described by equation (3.18). Equation (4.26) presents the quantity \( \mathbf{u} \cdot \nabla \hat{\mathbf{m}}_{\mid p} \) in linear basis form which can be readily computed, provided that the velocity vector \( \mathbf{u}_{p} \) for all nodes \( p \) is known or can be deduced.

In most problems, the voltage across device terminals driving the electric current is known. From the applied voltage, the current density throughout the device volume can be obtained by solving the homogeneous Poisson equation (Laplace’s equation) with corresponding boundary conditions (BCs)

\[
\sigma \nabla^{2} \phi = 0 \quad \text{(Laplace’s equation)}, \tag{4.27}
\]

\[
\nabla \phi \cdot \hat{\mathbf{n}} = 0 \quad \text{(BC for free boundaries)}, \tag{4.28}
\]

\[
\phi = f^{\text{BC}} \quad \text{(BC for contact boundaries)}.
\]

The electric potential is \( \phi \), \( \sigma \) is the electrical conductivity (assumed constant), and \( f^{\text{BC}} \) is the prescribed value of the potential at the boundaries. If the conductivity is not uniform, equation (4.27) should be replaced by \( \nabla \cdot (\sigma \nabla \phi) = 0 \).
To assist the discussion, we refer to the common example pictured in Fig. 4.4, consisting of a cylinder across whose ends a voltage is applied. The electrical potential at the left and right end are denoted by $\phi_L$ and $\phi_R$. The magnitude of the voltage applied across the device is thus $V = |\phi_R - \phi_L|$. The first expression (4.27) in the above equation set comes from the continuity condition, $\nabla \cdot \mathbf{J} = -\frac{\partial q}{\partial t}$, where $\mathbf{J} = \sigma \mathbf{E} = -\sigma \nabla \phi$, and $\frac{\partial q}{\partial t} = 0$ guarantees the absence of charge buildup in the system (i.e., at every instance the electrons are neutralized by the positive background charge of the conducting material).

Equation (4.27) can be expressed in the linear basis finite element representation as a set of equations for all mesh nodes $p \in [1, N]$,

$$\nabla^2 \phi = 0 \big|_{r_p} \rightarrow \sum_{l=1}^{M} \sum_{k=1}^{4} \Lambda_{(p)k}^l \phi_k^l = 0,$$

(4.30)

where $\Lambda_{(p)k}^l$ is the geometrical factor given by equation (4.25). As described in section 3.2.1, recasting $\Lambda_{(p)k}^l$ into a $N \times N$ matrix ($\Lambda_{(p)k}^l \rightarrow \Lambda$), leads to the discrete matrix-vector product representation of the Laplacian operation on a scalar quantity,

$$\nabla^2 \phi = 0 \rightarrow \mathbf{\Lambda} \mathbf{\phi} = \mathbf{0}.$$

(4.31)

In (4.31), $\mathbf{\Lambda}$ is the Laplacian matrix operator, and $\mathbf{\phi}$ is a vertical column vector whose scalar elements represent values of the electric potential at the mesh nodes, which are to be determined.

The second expression (4.28) in the equation set is a von Neumann boundary condition, ensuring that charge does not flow out of the system through the free boundaries. This boundary condition is implicitly included in the finite element representation of $\nabla^2 \phi = 0$ as described by (4.30) or (4.31) (section 3.2.1). Equation (4.31) can be expressed in matrix form as

$$\begin{pmatrix}
\Lambda_{11} & \Lambda_{12} & \cdots & \Lambda_{1N} \\
\Lambda_{21} & \ddots & & \\
\vdots & & \ddots & \\
\Lambda_{N1} & \cdots & & \Lambda_{NN}
\end{pmatrix}
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\vdots \\
\phi_N
\end{pmatrix}
= 
\begin{pmatrix}
0 \\
0 \\
\vdots \\
0
\end{pmatrix}.$$  

(4.32)
Incorporating in (4.32) the Dirichlet boundary condition (4.29) gives
\[
\begin{pmatrix}
\Lambda_{11} & \Lambda_{12} & \Lambda_{13} & \Lambda_{14} & \cdots & \Lambda_{1N} \\
0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 1 & 0 & \cdots & 0 \\
\Lambda_{41} & \Lambda_{42} & \Lambda_{43} & \Lambda_{44} & \cdots & \Lambda_{4N} \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
\Lambda_{N1} & \Lambda_{N2} & \Lambda_{N4} & \Lambda_{N5} & \cdots & \Lambda_{NN}
\end{pmatrix}
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\phi_4 \\
\vdots \\
\phi_N
\end{pmatrix}
= 
\begin{pmatrix}
0 \\
\delta_{2}^B \\
\delta_{3}^B \\
0 \\
\ddots \\
0
\end{pmatrix}.
\]
(4.33)

All off-diagonal matrix elements of \( \Lambda \) were set to 0, and the diagonal elements were set
to 1 in each row \( m \) where node \( m \) belongs to the contact boundary whose potential \( f_m^B \)
is given through the boundary condition (4.29). (Rows two and three in equation (4.33)
have been selected to be associated with the nodes located on the contact boundaries for
the purpose of exemplification.) To obtain the potential \( \phi_p \) at all mesh nodes \( p \) of the
tetrahedral mesh, one needs to solve the system of linear algebraic equations (4.33).

The generalized minimum residual method (GMRES) is an iterative method that
serves this purpose well [Saad and Schultz, 1986]. The first step in the procedure is
specifying an initial guess for \( \phi \). A common choice is the right-hand side of equation
(4.33). Once the initial guess is specified, the matrix-vector product \( \Lambda \phi_{\text{guess}} \) is computed
and passed together with the right-hand side of equation (4.33) to the GMRES subroutine.
The subroutine, after the first iteration, returns an arbitrary vector that is to be multiplied
by \( \Lambda \) and returned back to GMRES for an additional iteration. The iterative procedure
continues until \( \phi \) converges to the solution within a user-specified tolerance level.

Before calling the GMRES algorithm, however, it is prudent to ensure that the
order of magnitude of all nonzero matrix elements in (4.33) are as similar to each other
as possible to avoid unnecessary loss of computational accuracy due to round-off error.
Therefore, instead of using equation (4.33), we work with [Peterson et al., 1998]
\[
\begin{pmatrix}
\Lambda_{11} & \Lambda_{12} & \Lambda_{13} & \Lambda_{14} & \cdots & \Lambda_{1N} \\
0 & \tilde{\Lambda}_{(2)} & 0 & 0 & \cdots & 0 \\
0 & 0 & \tilde{\Lambda}_{(3)} & 0 & \cdots & 0 \\
\Lambda_{41} & \Lambda_{42} & \Lambda_{43} & \Lambda_{44} & \cdots & \Lambda_{4N} \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
\Lambda_{N1} & \Lambda_{N2} & \Lambda_{N4} & \Lambda_{N5} & \cdots & \Lambda_{NN}
\end{pmatrix}
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\phi_4 \\
\vdots \\
\phi_N
\end{pmatrix}
= 
\begin{pmatrix}
0 \\
\tilde{\Lambda}_{(2)} f_2^B \\
\tilde{\Lambda}_{(3)} f_3^B \\
0 \\
\ddots \\
0
\end{pmatrix}.
\]
(4.34)

The above equation is mathematically equivalent to (4.33). Factors \( \tilde{\Lambda}_{(m)} = \frac{1}{N} \sum_{i=1}^{N} \Lambda_{mi} \)
ensure a similar order of magnitude of all nonzero elements of \( \Lambda \). Passing the matrix-vector
product and right-hand side vector in equation (4.34) to a GMRES solver should yield, within several iterations, the electrical potential at all nodes $p$, for problems containing as many as hundreds of millions of unknowns. Once the potential at each node has been found, the electric field can be computed using

$$
E|_{r_p} = -\nabla \phi|_{r_p} \quad \rightarrow \quad E_p = -\sum_{l=1}^{M} \sum_{k=1}^{4} \nabla \xi^l_k \phi^l_k .
$$

(4.35)

With the electric field at all nodes $p$ known, the current density is obtained from

$$
J_p = \sigma E_p .
$$

(4.36)

Having obtained the expression for $J_p$, and hence $u_p = (1/M_s)(g \mu_B/2e)PJ_p$, we have all the ingredients to evaluate the adiabatic torque and nonadiabatic effective field. In the finite element representation, these are

$$
\tau_{STT, \text{adia}}^{\text{adia}}|_{r_p} = \frac{-1}{1 + \alpha^2} \left[ (u \cdot \nabla \hat{m}) + \alpha \hat{m} \times (u \cdot \nabla \hat{m}) \right]|_{r_p} \rightarrow
$$

$$
\tau_{p}^{\text{adia}} = \frac{-1}{1 + \alpha_p^2} \left[ \varsigma_p + \alpha_p \hat{m}_p \times \varsigma_p \right] ,
$$

(4.37)

and

$$
H_{\text{nonadia}}^{\text{STT}}|_{r_p} = \frac{-\beta}{\gamma} (u \cdot \nabla \hat{m})|_{r_p} \rightarrow H_p^{\text{STT, nonadia}} = \frac{-\beta_p}{\gamma} \varsigma_p ,
$$

(4.38)

where

$$
\varsigma_p = (u \cdot \nabla \hat{m})|_p = \sum_{l=1}^{M} \sum_{k=1}^{4} u_p \cdot \nabla \xi^l_k \hat{m}_k .
$$

(4.39)

We have decided in (4.39) to sum over all tetrahedrons, instead of over only those having node $p$ for a vertex (as done in (4.26)). Due to the local definitions of the linear basis functions, equations (4.39) and (4.26) are identical.

In conclusion, a linear basis finite element formulation of the adiabatic and nonadiabatic STT contribution to magnetization dynamics has been derived. The nonadiabatic contribution was cast in a field-like form that can be added to the effective field derivable from the variation of the micromagnetic free energy. The implementation of spin transfer torques presented here, the implementation of anisotropy, exchange, magnetostatics, and Zeeman fields presented in chapter 3, and numerical integration routines discussed in section 8.2, form the computational framework for simulating and investigating a wide range of magnetic phenomena, including current-driven domain wall motion in nanowires strips, domain wall pinning and depinning from notches in the presence of spin currents, and current-induced spin wave generation.
4.2.1 Point Contact Geometry

Various interesting physical phenomena have been identified by studying devices consisting of extended magnetoresistive multilayer stacks in contact with leads or pattern pillars through which currents are passed (Fig. 4.5). These phenomena include steady-state magnetization precession, spin-wave emission, vortex dynamics, and phase locking. In order to simulate magnetization dynamics in extended systems, it is necessary to know the current distribution throughout the device. This requires discretization of the entire system, and the solution of Laplace’s equation (4.27) with appropriate boundary conditions, in conjunction with a calculation of current redistribution due to magnetoresistive effects between the spacer-separated magnetic layers. For the case of a patterned spin valve structure, a simple procedure for the calculation of current redistribution was presented in section 4.1.1. A similar approach may be taken to approximate the local redistribution near the point contact(s) in extended devices. Once the current density throughout the device is known, the magnetization can be tracked via

\[
\frac{d\hat{m}_i}{dt} = -\frac{\gamma}{1 + \alpha_i^2} \left[ \hat{m}_i \times \left( \mathbf{H}_{\text{eff}}^i + \mathbf{H}_{\text{STT-int}}^i + \mathbf{H}_{\text{STT-cont, nonadia}}^i \right) 
+ \alpha_i \hat{m}_i \times \hat{m}_i \times \left( \mathbf{H}_{\text{eff}}^i + \mathbf{H}_{\text{STT-int}}^i + \mathbf{H}_{\text{STT-cont, nonadia}}^i \right) \right] + \tau_{\text{STT-cont, adia}}^i,
\]

where \(\mathbf{H}_{\text{eff}}^i\) denotes the effective field derivable from the micromagnetic free energy (section 2.2), \(\mathbf{H}_{\text{STT-int}}^i\) represents the field quantity accounting for the in-plane and out-of-plane STT contributions at the NM/FM interface (section 4.1), and \(\tau_{\text{STT-cont, adia}}^i\) and \(\mathbf{H}_{\text{STT-cont, nonadia}}^i\) account for the adiabatic (in-plane) and nonadiabatic (out-of-plane) torque contributions due to current flowing through regions of nonuniform magnetization within the ferromagnet (section 4.2).
4.2.2 Oersted Fields

In many geometries considered for STT applications, such as spin valve nanopillars and nanowires, the torques generated by Oersted (Amperian) fields are often significantly smaller than torques originating from the spin transfer torque effect, and are often ignored in micromagnetic calculations, since they are not expected to profoundly affect system response. However, the effects of Oersted fields are not always ascertainable in advance, and their inclusion in micromagnetic simulations is prudent. Including Oersted fields can in many cases help reveal subtle but important details that can affect device performance, such as modification of transition paths, turbulence in the motion of domain walls in nanowires, shifts in threshold currents or fields, and changes in dwell times associated with metastable states.

In other structures, such as laterally extended thin film vortex oscillators (section 12.1.4), Oersted fields can play a central role in device operation, and must be rigorously accounted for [Devolder et al., 2009]. Accurately representing Oersted fields is also important in modeling devices (or experimental setups) where current-carrying field-lines (which can be nonmagnetic) drive the magnetization (Fig. 4.6). This especially touches systems design, where quantitative results are sought and analytical approximations of the Oersted fields often fail to provide a realistic picture.

To obtain the Oersted field $\mathbf{H}_{OE}(\mathbf{r})$ generated by an electric current density $\mathbf{J}(\mathbf{r})$, we begin from the differential expression

$$\nabla \times \mathbf{H}_{OE} = \mathbf{J}. \quad (4.41)$$

Negating the existence of magnetic monopoles, $\nabla \cdot \mathbf{H}_{OE} = 0$, and we may write

$$\mathbf{H}_{OE} = \nabla \times \mathbf{A}, \quad (4.42)$$
with $A(r)$ being some vector potential. Substituting (4.42) into (4.41), one obtains

$$\nabla^2 A = - J,$$  

(4.43)

whence [Jackson, 1998]

$$A = \frac{1}{4\pi} \int \frac{J(r')}{|r - r'|} d^3 r'.$$  

(4.44)

Having the vector potential, we can readily evaluate the magnetic field using (4.42) as

$$H_{Oe}(r) = \frac{1}{4\pi} \nabla \times \int \frac{J(r')}{|r - r'|} d^3 r'.$$  

(4.45)

It remains to transcribe equation (4.45), given in continuum form, to a finite element linear basis expression. Since we are only interested in the Oersted field within the magnetic bodies, though the origins of the field may be currents passing through nonmagnetic regions of space (e.g., copper leads or field-lines), and considering that both magnetic regions and current-carrying nonmagnetic regions must be discretized for the evaluation of (4.45), it is convenient to be able to distinguish between the magnetic mesh and the nonmagnetic mesh. The former represents the observation domain and possibly all, or part of the source domain (in case of current passing through the magnetic region), and the latter represents exclusively a source domain. It is of further benefit to be able to make the distinction between the meshes of magnetic bodies supporting currents, and current-free magnetic bodies. The described distinctions can be achieved during the preprocessing stages prior to simulation by a separation of meshes approach or structured indexing. Assuming tetrahedral discretization of all magnetic bodies as well as current-carrying nonmagnetic bodies, the Oersted field at all nodes $p$ of the magnetic mesh can be expressed in linear basis representation (chapter 3) as

$$H_{Oe}^p = \frac{1}{4\pi} \nabla \times \sum_{l=1}^M \sum_{k=1}^4 \int_{V_l} \frac{\xi^l_k J^l_k}{|r_p - r'|} d^3 r',$$  

(4.46)

where $l$ runs over all $M$ tetrahedrons supporting a current, $k$ runs over the four vertices of each tetrahedron $l$, and the integral is taken over the volume of each tetrahedron, with position vector $r'$ being the dummy variable of integration, and position vector $r_p$ pointing to the coordinate of node $p$. If the integration region $V_l$ (source region) in the equation above is distant from the observation point $r_p$, it can be treated as a point source, so that the integral reduces to

$$\int_{V_l} \frac{\xi^l_k J^l_k}{|r_p - r'|} d^3 r' \simeq \frac{V_l}{4} \sum_{k=1}^4 \frac{J^l_k}{|r_p - r'_k|}$$ (far contribution) .  

(4.47)
Alternatively, the above integral can be evaluated to high accuracy using quadrature rules, as discussed elsewhere [Chang et al., 2011]. The described separation of the near and far field contributions follows the procedure for the computation of the magnetostatic field (section 8.1). Indeed, similarly as for the case of magnetostatics, direct computation of Oersted fields requires $O(\hat{M}N)$ operations, where $\hat{M}$ is the number of source nodes, and $N$ is the number of observation nodes. The size of both $\hat{M}$ and $N$ can be exceedingly large in many problems, posing a potential chokepoint for numerical computation. For this reason, the use of the nonuniform grid (NG) interpolation method (section 8.1.1) or the nonuniform fast Fourier transform (NUFFT) method (section 8.1.2) in conjunction with matrix-vector multiplication conducted on graphics processing units (GPUs) (section 8.3) is paramount for managing large problems, which, for certain systems of interest, can exceed hundreds of millions of unknowns.

Using the procedure outlined above, the Oersted field can now be evaluated and included in the effective magnetic field for the simulation of magnetization dynamics using the LLG equation, or one of its extensions,

$$H_{\text{eff}}^i = H_{\text{anis}}^i + H_{\text{ex}}^i + H_{\text{ms}}^i + H_{\text{Zee}}^i + H_{\text{Oe}}^i.$$ (4.48)
5 Modeling of Thermal Effects in Micromagnetics

In the present chapter we include thermal effects to the computational framework described in the previous two chapters. Langevin modeling based on the stochastic Landau-Lifshitz-Gilbert equation is described. Discretization criteria and numerical integration are discussed. Limitations of the model to resolve important features of magnetization response near the Curie point are pointed out. Landau-Lifshitz-Bloch micromagnetics is then introduced, which is the basis for simulations of heat assisted magnetic recording presented in chapter 10. Cases when modeling on the atomic scale is required are discussed.

5.1 Motivation

The preceding chapters focused on the modeling of magnetization dynamics in the absence of thermal effects. The presented equations describe the evolution of the magnetization under the deterministic influence of magnetic fields and spin polarized currents. This corresponds to the case of zero effective temperature, $T = 0$. Operating temperatures of most systems of interest (hard disk drives, magnetic random access memories, nanowire devices, etc.) are near room temperature. In case of heat assisted magnetic recording (HAMR), the operating temperatures can be as high as the Curie temperature or greater. When thermal effects are expected to qualitatively alter system response, or when the influence of thermal fluctuations on the noise levels, switching probabilities, or other system characteristics needs to be quantified, it is necessary to turn to a new framework that takes finite temperatures into account. The first model, discussed in section 5.2, extends the deterministic Landau-Lifshitz-Gilbert (LLG)
equation to include thermal fluctuations which are cast as random fields with temperature dependent amplitudes. The second model, described in section 5.3, allows for longitudinal magnetization relaxation and accounts for the temperature dependence of the susceptibility and other system parameters.

5.2 The Stochastic Landau-Lifshitz-Gilbert Equation

In order to model the effect of thermal fluctuations on magnetization dynamics, a random Gaussian white noise field $H_{th}$ with components uncorrelated in space and time is added to the deterministic field in the standard LLG equation (3.2), transforming it to the stochastic form

$$\frac{d\hat{m}}{dt} = -\frac{\gamma}{1 + \alpha^2} \hat{m} \times (H_{\text{eff}} + H_{th}) - \frac{\gamma\alpha}{1 + \alpha^2} \hat{m} \times \hat{m} \times (H_{\text{eff}} + H_{th}),$$

(5.1)

$$\langle H_{th,i}(r, t) \rangle = 0,$$

(5.2)

$$\langle H_{th,i}(r, t)H_{th,j}(r', t)\rangle = 2D\delta_{ij}\delta(r - r')\delta(t - t'),$$

(5.3)

$$D = \frac{\alpha}{1 + \alpha^2} \frac{k_B T}{\gamma M_s}.$$  

(5.4)

The subscript $i$ denotes one of the three spatial components in Cartesian coordinates, and $D$ is the noise power, derivable from the fluctuation dissipation theorem. In equation (5.4), $k_B$ is the Boltzmann constant, and $T(K)$ is the temperature. Equation (5.1) is perhaps the most commonly used equation for expressing the Langevin dynamics of magnetization under the influence of thermal fluctuations. However, alternative stochastic forms of the LLG equation also exist and are discussed in [Berkov, 2007].

Before we transform equations (5.1)–(5.4) to the finite element representation, we discuss the validity of the assumption that the components of the thermal field can be considered uncorrelated in both time and space. From a physical point of view, the fluctuations modeled by $H_{th}$ are due to interactions between the spins, phonons and electrons in the system. The timescales associated with processes of the latter two subsystems (equilibration times, phonon decay times, etc.) are less than a picosecond near room temperature [Berkov, 2007]. This is far below the characteristic time associated with the magnetization dynamics, which is given as the inverse of the precessional frequency ($\propto 1/\gamma H$). The disparity in the timescales warrants the adoption of the $\delta(t - t')$ correlator. The appearance of the spatial correlator $\delta(x - x')$ is justified by the fact that the typical
phonon wavelength near room temperature is only a few angstroms, well below the exchange length, and below the wavelengths of magnons of consequential amplitudes.

In discretized form, equations (5.1)–(5.4) read
\[
\frac{d\hat{m}_p}{dt} = -\frac{\gamma}{1 + \alpha_p^2} \hat{m}_p \times \left( H_{p}^{\text{eff}} + H_{p}^{\text{th}} \right) - \frac{\gamma \alpha_p}{1 + \alpha_p^2} \hat{m}_p \times \hat{m}_p \times \left( H_{p}^{\text{eff}} + H_{p}^{\text{th}} \right),
\]
(5.5)
\[
\langle H_{p,i}^{\text{th}}(t_m) \rangle = 0,
\]
(5.6)
\[
\langle H_{p,i}^{\text{th}}(t_m) H_{q,j}^{\text{th}}(t_n) \rangle = 2D_p \delta_{pq} \delta_{ij} \delta_{mn},
\]
(5.7)
\[
D_p = \frac{\alpha_p}{1 + \alpha_p^2} k_B T_p \frac{1}{\gamma M_s,p V_p \Delta t}.
\]
(5.8)

The above set of equations state that, at each time step during the numerical integration of the equation of motion (section 8.2), each spatial component of the thermal field $H_{p,i}^{\text{th}}$ on cell $p$ is drawn from a Gaussian distribution $\mathcal{N}(\mu, \sigma_p)$ characterized by mean $\mu = 0$ and standard deviation $\sigma_p = \sqrt{2D_p}$. In equation (5.8), $\Delta t$ represents the time step, and $V_p$ is the effective volume corresponding to node $p$, as given in equation (3.10). When modeling in the finite element linear basis representation of chapter 3, the subscript $p$ in (5.1)–(5.4) indicates a mesh node. In this case, $V_p$ represents the effective volume associated with the node $p$ as expressed in 3.10. For the case of Voronoi modeling, presented in chapter 7, the subscript $p$ in (5.1)–(5.4) denotes a Voronoi cell.

We take a moment to remark on the dependence of the thermal field amplitude on the volume $V_p$ and time step $\Delta t$, as expressed in equation (5.8). First, we note that in the limit when $V_p \to \infty$ or when $\Delta t \to \infty$, the thermal field is reduced to zero, $H_{p}^{\text{th}} \to 0$. This can be expected because, in the framework of finite elements, the thermal field $H_{p}^{\text{th}}$ acting on the magnetic moment within a finite volume $V_p$ during a time $\Delta t$ is just the volume and time average of the continuous thermal field $H_{\text{th}}(r)$, as described by equations (5.1)–(5.4). According to the zero spatial and temporal correlations, $H_{p}^{\text{th}}$ should average out to zero over the infinite volume $V_p \to \infty$, or the infinite time step $\Delta t \to \infty$, which is consistent with the occurrence of $V_p$ and $\Delta t$ in the denominator of equation (5.8).

From an atomistic perspective [Berkov, 2007], $H_{p}^{\text{th}}$ more closely represents the average thermal field over all spins within volume $V_p$, i.e., $H_{p}^{\text{th}} = \frac{1}{N} \sum_{s=1}^{N} H_{s}^{\text{th}}$, rather than the volume average of a continuous variable, $H_{p}^{\text{th}} = \frac{1}{V_p} \int_{V_p} H_{\text{th}}(r) \, dV$. Using the independence of random variables $H_{s}^{\text{th}}$, we have
\[
\langle H_{p}^{\text{th}^2} \rangle = \frac{1}{N^2} \sum_{s=1}^{N} \langle H_{s}^{\text{th}^2} \rangle.
\]
(5.9)
The statistical properties of $H_{s}^{th}$, being the same for each spin, allow us to replace $\sum_{s=1}^{N} \langle H_{s}^{th} \rangle$ with $N \langle H_{s}^{th} \rangle$ in the equations above to get

$$\langle H_{p}^{th} \rangle = \frac{1}{N} \langle H_{s}^{th} \rangle.$$  \hspace{1cm} (5.10)

Since the volume scales linearly with the number of spins in a system, the $1/N$ dependence in (5.10) reflects the $1/V$ dependence in equation (5.8).

Having described the form of the Langevin equation of motion for magnetization dynamics, we now discuss some important subtleties involving its numerical integration. In general, differential equations expressing stochastic processes, such as the equations (5.5)–(5.8), are only strictly defined once the rules of integration are specified. This is because different rules of integration result in different solutions to the stochastic problem. For systems with multiplicative noise, where a random variable is found in a product with system variables, such as in equation (5.5), the rules of integration imposed by the Stratonovich calculus lead to the correct result for the majority of systems governed by physical laws [Berkov, 2007].

If a stochastic differential equation is considered in the Stratonovich interpretation, the numerical integration scheme used to integrate the equation must reflect the rules of the Stratonovich calculus. The commonly used numerical integration schemes that coincide with the Stratonovich calculus are the Heun, Milstein, and the midpoint schemes.

Remarkably, due to the constraint of constant magnetization magnitude in the LLG equation, the Itô interpretation proves to be equivalent to the Stratonovich interpretation [Berkov and Gorn, 2002], expanding the limit of allowed numerical integration schemes. This equivalence does not hold for the case of the Landau-Lifshitz-Bloch equation of motion (section 5.3), where the magnetization magnitude is free to change, and adherence to the Stratonovich interpretation is required. Details of the implementation of different numerical schemes for the integration of deterministic and stochastic differential equations are given in section 8.2.

### 5.3 The Stochastic Landau-Lifshitz-Bloch Equation

In the previous section we extended the standard LLG equation valid for $T = 0$ to the stochastic form by introducing random terms to represent the fluctuating fields responsible for the Langevin dynamics. The strengths of these random fields were determined from statistical considerations in the context of the fluctuation-dissipation
theorem and the Fokker-Planck equation [Berkov, 2007]. However, it has been shown that the stochastic LLG equation, while adequately accounting for magnetization dynamics well below the Curie temperature $T_C$, does not reproduce some of the critical properties of the system near the Curie point. For example, the net equilibrium magnetization of a nanomagnet as a function of temperature is significantly misrepresented, and, as a consequence, the Curie temperature is grossly overestimated [Grinstein and Koch, 2003]. Other examples include the inability to properly compute reversal rates [Garanin and Chubykalo-Fesenko, 2004] and domain wall mobilities [Garanin, 1992] at temperatures close to $T_C$.

The reason the stochastic LLG equation fails to reproduce correctly the magnetization dynamics at elevated temperatures is because short wavelength excitations, which greatly contribute to the remagnetization and the demagnetization processes near $T_C$, are cut off due to the finite discretization of the magnetic body. This problem has been overcome by the derivation of a new equation of motion [Garanin et al., 1990], which endows the magnetization vector with a longitudinal degree of freedom, and interpolates between the Landau-Lifshitz equation and the Bloch equation. The Landau-Lifshitz-Bloch (LLB) equation has the form [Garanin, 1997]

$$\frac{d\mathbf{m}}{dt} = -\tilde{\gamma}\mathbf{m} \times \mathbf{H}_{\text{eff}} + \frac{\tilde{\gamma}\alpha_\parallel}{m^2} \mathbf{m} \cdot \left(\mathbf{H}_{\text{eff}} + \zeta_\parallel\right) \mathbf{m} - \frac{\tilde{\gamma}\alpha_\perp}{m^2} \mathbf{m} \times \mathbf{m} \times \left(\mathbf{H}_{\text{eff}} + \zeta_\perp\right), \quad (5.11)$$

where $\mathbf{m} = \mathbf{M}/M_e^0$ is the normalized magnetization vector and $M_e^0 = M_e(T = 0)$ is the spontaneous equilibrium magnetization at absolute zero. The longitudinal and transverse damping parameters, $\alpha_\parallel$ and $\alpha_\perp$, are given by

$$\alpha_\parallel = \lambda \frac{2T}{3T_C}, \quad \alpha_\perp = \left\{ \begin{array}{ll} \lambda \left(1 - \frac{T}{3T_C}\right) & , \quad T < T_C, \\ \lambda \frac{2T}{3T_C} & , \quad T \geq T_C, \end{array} \right., \quad (5.12)$$

where $T$ is the temperature, $T_C$ is the Curie temperature, and $\lambda$ denotes the dimensionless damping parameter quantifying the coupling of the spins to the thermal bath. Finally, $\tilde{\gamma}$ in (5.11) denotes the normalized gyromagnetic ratio, expressed as $\tilde{\gamma} = \frac{\gamma}{1 + \lambda T}$.

The effective field in equation (5.11) is obtained as the variational derivative of the energy density with respect to the magnetization, $\mathbf{H}_{\text{eff}} = -\delta \varepsilon / \delta \mathbf{M}$, where $E = \int_V \varepsilon dV$ is the energy derived from mean-field theory [Garanin, 1997]

$$E = \int_V \left[ -\mathbf{H}_{\text{app}} \cdot (M_e^0 \mathbf{m}) + A (\nabla \mathbf{m})^2 + \frac{(M_e^0)^2}{2\chi_\perp} m_\perp^2 + \frac{1}{8m_e^2\chi_\parallel} (m^2 - m_e^2)^2 \right], \quad (5.13)$$
\[ H_{\text{eff}} = H_{\text{app}} + \frac{2A}{M_e^0} \nabla^2 m - \frac{m_e^2}{\chi_{\perp}} + \begin{cases} \frac{1}{2\chi_\parallel} \left( 1 - \frac{m_e^2}{m_e^0} \right) m, & T < T_C, \\ \frac{1}{\chi_{\perp}} \left( 1 - \frac{3T_C m_e^2}{5(T-T_C)} \right) m, & T \geq T_C, \end{cases} \quad (5.14) \]

Here, \( \tilde{\chi}_\mu = \frac{\partial m}{\partial H} \bigg|_{H \to 0} \) are the longitudinal (\( \mu = \| \)) and transverse (\( \mu = \perp \)) susceptibilities, \( m_e(T) = \frac{M_e(T)}{M_e^0} \) is the normalized spontaneous magnetization at temperature \( T \). Use of the relation \( M_e^2 \propto \frac{1}{\chi_\parallel} \propto 1 - \frac{T}{T_C} \) has been made in extending the last integrand term in equation (5.13) to \( T > T_C \) [Garanin, 1997].

The stochastic terms in equation (5.11), used to model thermal fluctuations, are

\[ \langle \zeta_\mu^i(r,t) \rangle = 0, \quad (5.15) \]

\[ \langle \zeta_\mu^i(r,t) \zeta_\nu^j(r',t') \rangle = \frac{2k_B T}{\gamma \alpha_\| M_e^0} \delta_{\mu\nu} \delta_{ij} \delta(r-r') \delta(t-t'). \quad (5.16) \]

As before, \( \mu \) and \( \nu \) denote \( \| \) or \( \perp \), while \( i \) and \( j \) indicate the three spatial components. Lastly, \( \zeta_\mu^i(r,t) \) represents a Gaussian white-noise random variable whose variance was determined from the fluctuation-dissipation theorem.

It is worth commenting on several properties of the LLB equation, as expressed in (5.11). As seen from preceding expressions, the LLB equation is defined over the entire range of temperatures, below and above \( T_C \). The magnetization is no longer constrained, but allowed to vary. The second term in equation (5.11) expresses the longitudinal relaxation of the magnetization, modulated by the longitudinal damping parameter \( \alpha_\| \). The temperature dependence of the longitudinal and transverse damping parameters are given in (5.12). The temperature dependence of the quantities \( m_e(T), \chi_\parallel(T), \chi_\perp(T) \), and \( A(T) \) can be approximated from a mean-field approach, or obtained from atomistic simulations [Kazantseva et al., 2008], the topic of the upcoming section.

We note that, as for the case of the stochastic LLG equation, the introduction of stochastic terms in the LLB equation is not unique. Different stochastic formulations of the LLB equation can lead to different solutions, the difference between which can be particularly pronounced near the Curie point. The stochastic LLB equation, as formulated in (5.11), has been shown to correctly resolve many of the characteristics of magnetic systems, which are misrepresented by simulations based on the stochastic LLG equation, such as high-temperature transverse and longitudinal relaxation rates [Chubykalo-Fesenko et al., 2006a] and the temperature dependence of domain wall structure [Hinzke et al., 2007, Hinzke et al., 2008]. However, the equilibrium solution
to equation (5.11) in the vicinity of $T_C$ was shown not to satisfactorily reproduce the expected Boltzmann distribution. An alternative more robust formulation that meets this equilibrium requirement has been recently proposed [Evans et al., 2012],

$$\frac{dm}{dt} = -\gamma m \times H_{\text{eff}} + \frac{\gamma \alpha_\parallel}{m^2} (m \cdot H_{\text{eff}}) m - \frac{\gamma \alpha_\perp}{m^2} m \times m \times (H_{\text{eff}} + \zeta_\perp) + \zeta_\parallel,$$  \hspace{1cm} (5.17)

$$\left\langle \zeta_\parallel(L)(r,t) \right\rangle = 0,$$  \hspace{1cm} (5.18)

$$\left\langle \zeta_\parallel_j(r,t) \zeta_\parallel_j^i(r',t') \right\rangle = \frac{2k_B T (\alpha_\parallel - \alpha_\parallel)}{\gamma M_0^2 \alpha_\perp} \delta_{ij} \delta(r - r') \delta(t - t'),$$  \hspace{1cm} (5.19)

$$\left\langle \zeta_\parallel_i(r,t) \zeta_\parallel_j(r',t') \right\rangle = \frac{2\gamma k_B T \alpha_\parallel}{M_0^2} \delta_{ij} \delta(r - r') \delta(t - t'),$$  \hspace{1cm} (5.20)

$$\left\langle \zeta_\parallel_i(r,t) \zeta_\parallel_j^i(r',t') \right\rangle = 0.$$

The above stochastic form of the LLB equation was proven to be consistent with both the fluctuation-dissipation theorem and the Fokker-Planck equation near $T_C$ [Evans et al., 2012].

In section 5.2, it was noted that the stochastic LLG equation could be considered in either the Stratonovich or Itô interpretation, with no consequence on the physical solution. This was because the Stratonovich and Itô interpretations happen to be equivalent for the case of the stochastic LLG equation, owing to the fixed magnetization length [Berkov and Gorn, 2002]. In the case of the stochastic LLB equation, given in (5.11) or (5.17), the constraint of constant magnetization magnitude no longer holds, and the stochastic differential equation only becomes strictly defined once the stochastic calculus is specified. As for the majority of systems governed by physical laws, the stochastic LLB equation warrants the adoption of the Stratonovich calculus. This places a constraint on the type of numerical integration schemes which are allowed for obtaining a solution to the Langevin dynamics. Examples of numerical methods that obey the rules of Stratonovich calculus include Heun’s method, midpoint formula, and Milstein schemes.

Implementation of the stochastic LLB equation in the framework of the linear basis finite element method (chapter 3) or Voronoi modeling (chapter 7) involves the transformation of the continuous variables, $m(r,t), H_{\text{eff}}(r,t)$, and $\zeta^\mu(r,t)$ and continuous parameters $\gamma(r), \alpha_\parallel(r), \alpha_\perp(r), \chi_\parallel(r), \chi_\perp(r), m_e(r)$, and $A(r)$ to a discretized form. For the fields, this implies the transcription $m(r,t) \rightarrow m_p, H_{\text{eff}}(r,t) \rightarrow H^p_{\text{eff}},$ and $\zeta^\mu(r,t) \rightarrow \zeta^\mu_p$, where in (5.15) and (5.16), or (5.18)–(5.21), the Dirac delta functions transcribe as $\delta(r - r') \rightarrow \delta_{pq}/V_p$ and $\delta(t - t') \rightarrow \delta_{mn}/\Delta t$. The indices $p$ and $q$ represent
nodes of the tetrahedral mesh in the case of linear basis finite element modeling, or Voronoi cells in the case of Voronoi modeling, while indices \( m \) and \( n \) indicate times \( t_m \) and \( t_n \), and \( \Delta t \) is the time step taken in the numerical integration of the Langevin equation of motion. The continuous parameters forgo their spatial dependence and become nodal coefficients \( \tilde{\gamma}(\mathbf{r}) \rightarrow \tilde{\gamma}_p \), \( \alpha_\perp(\mathbf{r}) \rightarrow \alpha_{\perp,p} \), \( \chi(\mathbf{r}) \rightarrow \chi_{\parallel,p} \), \( \chi_\perp(\mathbf{r}) \rightarrow \chi_{\perp,p} \), \( m_e(\mathbf{r}) \rightarrow m_{e,p} \), and \( A(\mathbf{r}) \rightarrow A_p \). The temperature dependence of \( \chi_{\parallel}(T) \), \( \chi_{\perp}(T) \), \( m_e(T) \), and \( A(T) \) can be assigned an analytical form or provided as tabulated input obtained from atomistic simulations.

### 5.4 Atomistic Modeling

While micromagnetics provides a precious framework for the study of magnetization dynamics for a variety of systems of interest, as evidenced by the simulation results presented in chapters 9–13, in specific cases, standard macroscopic assumptions prevent key features of magnetization response to be computationally reproduced, faithfully, or at all. Laser pulse-induced demagnetization and remagnetization processes are one such example [Kirilyuk et al., 2010].

To broaden the scope of physical processes accessible by micromagnetics, the LLG equation was modified to allow for longitudinal relaxation. This new equation is called the Landau-Lifshitz-Bloch (LLB) equation, and was the topic of the previous section. As had been there noted, magnetic moment density \( M_e(T) \), transverse and longitudinal susceptibilities \( \chi_\perp(T) \), \( \chi_{\parallel}(T) \), and the exchange stiffness parameter \( A(T) \) enter LLB micromagnetics as parameterized input provided by atomistic simulations and/or mean-field theory calculations. The present section is dedicated to atomistic simulations, which serve not only for parametrization purposes, but are also of value in resolving certain features of interest which LLG and LLB micromagnetics may fail to capture.

Atomistic modeling begins with the Heisenberg Hamiltonian,

\[
H_i = -\sum_{j\neq i} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j,
\]

where \( \mathbf{S}_i \) is the atomic spin at site \( i \), \( j \) runs over all other spin sites, and \( J_{ij} \) denotes the exchange integral for spins indexed \( i \) and \( j \). Since \( J_{ij} \) can be non-vanishing even for neighbors several lattice spacings away, the exchange field in atomistic modeling can bear
a long-range character. This is in contrast to micromagnetic modeling, where only nearest-neighbor interactions are included. Hence, in atomistic modeling, where the materials of interest typically have a regular lattice or several regular sublattices, the exchange field may be effectively lumped together with the dipolar field, and evaluated efficiently at each simulation time step using the FFT method (section 8.1). The magnetocrystalline anisotropy, Zeeman energy, and other terms are included with the exchange term in the full spin Hamiltonian from which the effective magnetic fields can be derived. The full Hamiltonian for the L10 FePt alloy extensively investigated for magnetic recording applications is given in [Mryasov et al., 2005].

Once the effective magnetic fields are evaluated at each atomic site, the LLG equation may be used to track the dynamic evolution of spins, or relax the system to an equilibrium configuration, just as in micromagnetic simulations. More significantly, including stochastic thermal fields to the LLG equation, as done in section 5.2, allows the determination of the temperature dependence of $M_e(T)$, $\chi_{\perp}(T)$, $\chi_{\parallel}(T)$, and $A(T)$ [Kazantseva et al., 2008]. Figure 5.1 illustrates a typical decay of macroscopic magnetization of a nanoparticle as the temperature is elevated. At $T = 0$, all atomic spins are aligned, and the moment density is known from ab initio calculations. At finite temperatures, the macroscopic density is computed by averaging over many atomic spins. The Curie temperature is deduced this way.

Spin modeling on the atomic scale further allows the study of nonequilibrium
processes such as disorder dynamics following a sudden temperature spike induced by a high-fluence laser pulse. Atomistic simulations were shown to correctly reproduce longitudinal and transverse relaxation times associated with equilibration [Chubykalo-Fesenko et al., 2006b, Kazantseva et al., 2008]. The failure of LLG-based micromagnetic simulations to resolve demagnetization and remagnetization processes is due to the lack of representation of short wavelength excitations in the spin wave spectrum – a consequence of macroscopic discretization. This failure served as motivation for the derivation of the LLB equation, which, when supplied by needed information from atomistic simulations, can implicitly account for short-wavelength excitations through longitudinal relaxation and can reproduce demagnetization and remagnetization processes well.

Atomistic simulations help reveal other features inaccessible to micromagnetics alone. For the ordered L1$_0$ FePt system, the spin Hamiltonian is modified to account for the exchange-induced Pt magnetic moment, and appropriately treats the Fe spins as the only independent degrees of freedom [Mryasov et al., 2005]. Atomistic simulations based on this Hamiltonian show that the domain wall width depends on the orientation of the domain wall with respect to the lattice structure [Hinzke et al., 2007]. This is due to the anisotropic nature of exchange interactions in the layered L1$_0$ FePt. Atomistic simulations also reveal that the domain wall type changes from circular, to elliptical, to linear, as temperature is increased [Hinzke et al., 2008]. These transitions of domain wall type with temperature in L1$_0$ FePt have also been reproduced by LLB simulations.

Other cases where atomic resolution is desirable is in the modeling of ferromagnetic and antiferromagnetic materials and complex heterostructures in which the atomic spin magnitude and sign of the exchange integral may oscillate from one lattice site to the next. Such systems are inaccessible to micromagnetic modeling due to the presumed continuity of magnetization within discretization cells encompassing many atomic spins. Similarly desirable is atomic resolution in the modeling of nanoislands for patterned media application where bits may be only several atomic layers in dimension. In such cases atomistic modeling may be used to help resolve the effects of surface strain and defects introduced by the patterning process, which are considered to be capable of destroying reversal coherence of nanoislands as small as 5 nm in size. Atomistic simulations were also shown to be able to more truthfully portray domain wall compression and injection through interfaces in systems such as FePt/FeRh when interlayer exchange coupling is weak [Phuoc et al., 2007].
Finally, as pointed out in [Kazantseva et al., 2008], since zero-temperature properties enter atomistic modeling from first principles calculations, and since atomistic simulations can provide the needed parametrization for LLB dynamics, fitting parameters need not enter at any level of computation. The firm link between ab initio calculations at the electronic level, atomistic spin modeling, and macroscopic modeling based on LLB micromagnetics sets stage for multiscale computation where calculations at different regions or instances can be performed on different levels and interfaced with one another consistently. Multiscale modeling thus offers a holistic approach to spin dynamics in complex materials systems and structures, and is accommodating to a diverse range of interactions and phenomena, including spin/charge transport and accumulation, magnetoresistance effects, and spin transfer torques.
6 Techniques for Calculating Energy Barriers in Micromagnetics

This chapter summarizes several existing numerical techniques for the calculation of transition rates and energy barriers in micromagnetics. Stochastic methods are first considered. Their limitations and extensions are described. The nudge elastic band method is then presented, which allows for the deterministic calculation of energy barriers [Escobar et al., 2012a]. Constrained versus unconstrained differentiation of the energy with respect to the magnetization is discussed in reference to the Landau-Lifshitz-Gilbert equation. Improvements to the initial guess path are analyzed. The nudge elastic band method presented here enabled the computation of energy barriers for Co/Pd multilayer islands and magnetically frustrated nanorings analyzed in chapters 11 and 13.

6.1 Stochastic Methods

In the previous chapter we have illustrated procedures of simulating magnetization dynamics in presence of thermal agitation using Langevin dynamics. The utility of the described stochastic methods is demonstrable in computational studies of signal fluctuations in GMR and TMR sensors (section 12.1.1), spectral linewidth broadening in spin-torque nanooscillators (section 12.1.4), switching probability distributions and correlations to switching times in spin valves (section 12.1.2), and reversal mode and thermal stability analysis in magnetic memory technologies, including granular recording media (chapter 9), bit patterned media (chapter 11), magnetic random access memories (chapter 12), and domain wall-based memory and logic devices (chapter 13). In this
section, we highlight the utility of stochastic methods for the determination of transition rates, energy barriers, and reversal modes.

Since micromagnetic simulations incorporating Langevin dynamics provide a satisfactory description of realistic magnetization behavior for many cases of interest, we may endeavor to perform a series of simulations in order to obtain the necessary statistics to deduce transition rates, modes of reversal, and minimum energy barriers associated with events such as thermally induced magnetization switching of a perpendicular magnetic anisotropy nanoisland, or domain wall depinning from an artificial notch. Unfortunately, the processing power of today’s computational hardware, even when enhanced by massively parallelized GPU architectures (section 8.3), still comes substantially short of simulating thermal activation processes over energy barriers of order $\sim 1 \, k_B T$ or greater, even for the smallest of problem sizes. Considering that thermally activated processes of greatest importance to the development of future generation memory technologies are those associated with transitions over energy barriers of $\sim 50 \, k_B T$ (corresponding to $\sim 10$ years of thermal stability), direct Langevin simulations as a tool for the investigation of such events are impracticable. Alternative techniques must therefore be developed to help us infer transition rates and energy barriers for systems of greatest interest.

### 6.1.1 Extrapolation Methods

For the calculation of transition rates over large energy barriers, one might consider extrapolation methods relying on the Arrhenius-Neé law (section 2.1.9)

$$\tau = \tau_0 \exp \left( \frac{E_b}{k_B T} \right). \quad (6.1)$$

Numerical simulations may thus first be employed to obtain transition rates over energy barriers that are sufficiently small to render computation feasible. Subsequently, the acquired data may be used to extrapolate to higher energy barriers and longer transition times. Reduced energy barriers required for the first part of the method can be achieved by application of an applied field, for example. Due to the large differences between timescales accessible by simulations and those characteristic of thermally activated processes over large energy barriers, the results of the outlined approach are generally unconvincing due to extrapolation over several orders of magnitude [Dittrich, 2003].
6.1.2 Time-Temperature Equivalence Method

Another approach for obtaining results pertaining to prolonged processes in reduced computational time is based on the semblance of a time-temperature equivalence [Xue and Victora, 2000]. The approach stems from the tentative observation that transitions over a given energy barrier at low thermal agitation are similar in character to transitions at high thermal agitation, apart from the rates of incidence. The method relies on equation (6.1), from which we have

\[ k_B T \log \left( \frac{\tau}{\tau_0} \right) = k_B T' \log \left( \frac{\tau'}{\tau_0} \right), \]

(6.2)

since we are considering a single energy barrier \( E_b = E'_b \). The method assumes \( \tau_0 = \tau'_0 \) for the entire range of temperatures entering considerations. The idea is to simulate Langevin dynamics at a much elevated temperature \( T' \gg T \), in order to emulate processes described by a characteristic time \( \tau \) on a much shorter timescale \( \tau' \). To obtain the attempt time \( \tau_0 \), the temperature \( T \) is first chosen such that the corresponding timescale \( \tau \) for some chosen process of consideration is still accessible computationally. After simulations at temperatures \( T \) and \( T' \), values \( \tau \) and \( \tau' \) may be deduced, and \( \tau_0 \) can be obtained from equation (6.2). Having computed the attempt time, it becomes possible to simulate magnetization dynamics at some artificially elevated temperature \( T'' \), under a substantially reduced characteristic time \( \tau'' \), and reasonably well reproduce dynamical features occurring over \( \tau \gg \tau'' \) at temperature \( T \ll T'' \), for many problems of interest. The success of the time-temperature equivalence method has been demonstrated in computations of MH loops at different temperatures and sweep rates [Xue and Victora, 2000], as well as in simulations of thermally induced bit decay over long time scales [Xue and Victora, 2001].

6.1.3 Other Stochastic Methods

Other variants of stochastic methods for the determination of transition rates, attempt frequencies, decay/reversal modes, and energy barriers have been developed. Some of these include hybrid methods involving forward flux sampling [Vogler et al., 2011], semi-analytical methods extended by kinetic Monte Carlo simulations [Parker and Hitchon, 2012], and methods based on the relation between temperature, transition probability as a function of bias, and the Arrhenius-Neél relation [Zhu and Kang, 2012].
6.2 Nudged Elastic Band Method

Alternative routes exist for the determination of energy barriers and estimation of transition rates that do not rely on the direct simulation of Langevin dynamics. These include the path integral method, the string method, and the nudged elastic band method (NEBM) [Berkov, 2007]. These methods all involve a path finding scheme which yields a transition path connecting two micromagnetic states across the lowest existing energy barrier in configuration space. The common advantage of the methods is that the evaluation of the energy barrier is deterministic (apart from the possible degeneracy of the solution space). This is in contrast to the stochastic approaches of the preceding section, where multiple simulation runs and averaging over different magnetization trajectories are necessary. Further in contrast, the computational cost for the path finding methods does not increase with the energy barrier height, which is particularly advantageous for studying stability of magnetic memory devices with very large energy barriers. The present section provides a description of the NEBM as implemented in [Escobar et al., 2012a]; cf. [Dittrich et al., 2002]. Results of energy barrier calculations using the NEBM can be found in sections 11.4.3, 11.3, and 13.2.

6.2.1 Finding the Minimum Energy Path

The aim of the NEBM is to find the minimum energy path (MEP) connecting two magnetization states in configuration space [Jónsson et al., 1998]. The MEP obtained by the NEBM is a discretized representation of a continuous evolution of magnetization from the initial to the final state (Fig. 6.1). The discretized representation is in the form of a sequence of images, each representing the magnetization configuration at a particular point along the transition path.

If we assume the path is discretized by \( n \) images (Fig. 6.1), then for each image \( k \in [1, n] \) the magnetization configuration of the system can be described by a composite vector \( \mathbf{m}^k \) which stores the unit moment vectors \( \hat{\mathbf{m}}_i^k \) at all nodes \( i \in [1, N] \) of the finite element tetrahedral mesh, i.e., \( \mathbf{m}^k = (\hat{\mathbf{m}}_1^k \hat{\mathbf{m}}_2^k \ldots \hat{\mathbf{m}}_N^k) \). In other words, knowing \( \mathbf{m}^k \) one fully knows the state of the system at image \( k \). To begin with the calculation of the energy barrier using the NEBM, a guess path needs to be provided, which will eventually converge to the MEP during the path finding procedure. The guess path is provided by specifying \( \mathbf{m}^k \) for all images \( k \in [1, n] \). Often enough, for simple problems, a satisfactory route to specifying the guess path is to linearly interpolate between the initial and final
Figure 6.1: Transition paths represented by a sequence of images: (a) coherent reversal of a perpendicular magnetic anisotropy nanodisk; (b) field-induced reversal; (c) reversal along the minimum energy path.

states, $\mathbf{m}^1$ and $\mathbf{m}^n$, to obtain $\mathbf{m}^k$ for $k \in [2, n - 1]$ (Fig. 6.1a).

If the energy landscape is complex, with many extrema and saddle points, a more sophisticated guess path is required in order to help avert convergence to an unsought transition path and/or avoid long search times. An improved guess path can be obtained by simulating magnetization dynamics (using the LLG equation) under an applied field chosen to lead to the transition from the initial to the final state $\mathbf{m}^1 \rightarrow \mathbf{m}^n$. Configurational excerpts from the transition $\mathbf{m}^1 \rightarrow \mathbf{m}^n$ can then be used to populate $\mathbf{m}^k$ for $k \in [2, n - 1]$. The guess path thus obtained (Fig. 6.1b) is more likely to resemble the MEP (Fig. 6.1c) than the guess path obtained by linear interpolation between the end images (Fig. 6.1a), and the convergence to the solution proceeds in shorter time [Dittrich et al., 2002, Suess et al., 2005]. An alternative scheme for obtaining guess paths is considered in section 6.2.4.

Once the guess path is obtained, the iterative path finding procedure can be performed. This procedure consists of moving each image $k$ along the direction normal
to the path, according to
\[
\frac{d\mathbf{m}^k}{d\xi} = -\left[ \nabla^c_{\mathbf{m}} E|_{\mathbf{m}^k} - \left( \nabla^c_{\mathbf{m}} E|_{\mathbf{m}^k} \cdot \hat{\mathbf{t}}^k \right) \hat{\mathbf{t}}^k \right],
\]
(6.3)
or, equivalently,
\[
\frac{d\mathbf{m}^k}{d\xi} = \hat{\mathbf{t}}^k \times \hat{\mathbf{t}}^k \times \nabla^c_{\mathbf{m}} E|_{\mathbf{m}^k},
\]
(6.4)
where \(\xi\) is the dummy integration parameter, \(E(\mathbf{m})\) is the energy functional, \(\nabla^c_{\mathbf{m}}\) is the gradient with respect to \(\mathbf{m}\), the superscript \(c\) indicating that the differentiation is constrained (in reverence of \(|\hat{\mathbf{m}}_i| = 1\) for each vector element \(i\) of \(\mathbf{m}\)), the vertical bar \(|m^k|\) means evaluated at \(\mathbf{m}^k\), and \(\hat{\mathbf{t}}^k\) is the local unit tangent vector directed along the path at image \(k\), specified by

\[
\hat{\mathbf{t}}^k = \begin{cases} 
\frac{\mathbf{m}^{k+1} - \mathbf{m}^k}{|\mathbf{m}^{k+1} - \mathbf{m}^k|}, & E(\mathbf{m}^{k-1}) < E(\mathbf{m}^k) < E(\mathbf{m}^{k+1}), \\
\frac{\mathbf{m}^{k-1} - \mathbf{m}^k}{|\mathbf{m}^{k-1} - \mathbf{m}^k|}, & E(\mathbf{m}^{k-1}) > E(\mathbf{m}^k) > E(\mathbf{m}^{k+1}), \\
\frac{\mathbf{m}^{k+1} - \mathbf{m}^{k-1}}{|\mathbf{m}^{k+1} - \mathbf{m}^{k-1}|}, & E(\mathbf{m}^{k-1}) < E(\mathbf{m}^k) > E(\mathbf{m}^{k+1}),
\end{cases}
\]
(6.5)

The conditional definition of \(\hat{\mathbf{t}}^k\) given above has been shown to noticeably eliminate kinks in the energy path that can develop as an artifact of the numerical procedure [Henkelman and Jonsson, 2000]. It is important to avoid kinks in the energy path because they can cause the iterative procedure to oscillate indefinitely between two intermediate solutions and prevent convergence to the MEP. For convergent problems, Jacobian-enhanced solvers can greatly accelerate the iterative algorithm to allow the solution to be reached in fewest number of steps. A new implementation of an analytical-based Jacobian-enhanced NEBM solver can be found in [Escobar et al., 2012a].

In order to ensure uniform spacing between the images, a spring-like contribution is often added to equation (6.3), or (6.4), giving
\[
\frac{d\mathbf{m}^k}{d\xi} = \hat{\mathbf{t}}^k \times \hat{\mathbf{t}}^k \times \nabla^c_{\mathbf{m}} E|_{\mathbf{m}^k} + k_s \left( |\mathbf{m}^{k+1} - \mathbf{m}^k| + |\mathbf{m}^k - \mathbf{m}^{k-1}| \right) \hat{\mathbf{t}}^k,
\]
(6.6)
where \(k_s\) is the spring constant. Equation (6.6), with the unit tangent vector as defined in (6.5), has been shown to minimize kinks and eliminate corner cutting and image collapse, thus leading to improved convergence [Henkelman and Jonsson, 2000]. The magnitude of
the spring force can be varied by orders of magnitude without affecting convergence to the correct solution [Dittrich et al., 2002].

6.2.2 Evaluation of the Energy Gradient

We now turn to the evaluation of the energy gradient $\nabla_m E$ necessary for the integration of equation (6.6). It is important to note that the gradient $\nabla_m E$ represents the constrained differentiation with respect to $m$ regardful of $|\hat{m}_i^k| = 1$. That we are working with the constrained differentiation operator is reasonable, considering that we are searching for the MEP over an energy landscape that is a layout of all physically realizable magnetization configurations subject to $|\hat{m}_i^k| = 1$ (section 2.1). The constrained gradient of the energy functional can be simply written as

$$\nabla_m E = -m \times m \times \nabla m E,$$  \hspace{1cm} (6.7)

where $\nabla m E$ is the unconstrained energy gradient through which we can express the effective field according to (2.47). The effective micromagnetic field at node $i$ of image $k$ is given as

$$H_{i}^{\text{eff}}(m^k) = -\frac{1}{M_{s,i}V_i} \frac{\delta E}{\delta \hat{m}_i^k} \bigg|_{m^k}.$$  \hspace{1cm} (6.8)

Hence, for each vector element $i \in [1, N]$ of vector $\nabla_m E$ we have

$$(\nabla_m E|_{m^k})_i = M_{s,i}V_i \hat{m}_i^k \times \hat{m}_i^k \times H_{i}^{\text{eff}}(m^k).$$  \hspace{1cm} (6.9)

With all quantities and expressions known, including $H_{i}^{\text{eff}}(m^k)$ from chapter 3, it is now possible to numerically integrate (6.6) in order to obtain the MEP. Details of the numerical integration are provided in section 8.2.

6.2.3 Fixed versus Loose Ends Approach

So far we have considered images 1 and $n$ fixed, i.e., only the magnetization configurations of images 2 to $n - 1$ were allowed to evolve in equation (6.6). Once the numerical integration of equation (6.6) has converged, the MEP, corresponding to the transition between the initial and final image, is found (Fig. 6.2). The maximum point in the MEP represents the saddle point of the energy landscape. The difference between the energy of the first image and the highest point on the MEP represents the barrier for the given transition in the forward direction (from initial to the final state; see section
Figure 6.2: Transition between two stable states of a perpendicular magnetic anisotropy nanodisk along the minimum energy path discretized by 10 images, showing the energy at each image.

11.4.3 for asymmetric barrier). This barrier can then be used to estimate the associated transition rate according to (2.38).

However, to calculate the barrier between two stable states using the NEBM with fixed end images, it is important that the first and last images represent the equilibrium magnetization configurations of the system in the two respective stable states. This implies that the LLG equation must be simulated twice in order to obtain the two needed equilibrium configurations before the NEBM can be employed. This is conventionally done by initializing the system in some state similar to the expected equilibrium state and allowing it to relax to equilibrium. Initialization usually involves setting the magnetization of the entire structure to point homogeneously in a given direction. This approach is well suited when the system in consideration is a uniaxial nanomagnet that has two stable states, “up” and “down”. Relaxing such a system from an initial state with the magnetization perfectly pointing along the vertical direction will allow the moment vectors at the top and bottom surfaces to slightly fan in/out (due to magnetostatic interactions) and reach equilibrium. For more complicated systems, with more complex
stable configurations, the magnetization at the different regions of the structure may be initialized independently from one another. Additionally, an applied field may be used to assist the transition to the desired equilibrium state. This is important for the preparation of vortex states in nanodisks, where four distinct states can be achieved depending on the combination of chirality and polarity values.

When the applied field is not needed for the preparation of the equilibrium state, and relaxation from a homogeneous (or piecewise homogeneous) configuration suffices, simulations of the LLG equation prior to the NEBM can be avoided by allowing the end images in the NEBM to be loose, i.e., allowing the magnetization configuration of all images 1 through \( n \) to evolve. Though this increases the number of unknowns from \( 3N(n-2) \) to \( 3Nn \), it enables the end images to converge to the nearest energy minimum, so that the transition barrier between the two stable states can be conveniently deduced from the converged MEP in one run, with no need of independent initial and final state preparation.

For the implementation of the loose ends approach, it is important to evolve the end images without the tangential components in (6.6), and without the spring force contribution, i.e., simply by

\[
\frac{dm^k}{d\xi} = -\nabla_c E |_{m^k} \quad \text{for } k = 1 \text{ or } n ,
\]  

which can be recognized as the LLG equation without the precessional term, and normalized damping (see (6.9)). Equation (6.10) guarantees that the convergence of the end images to the local energy minimum is unaffected by the magnetization configurations of the intermediate images.

It can be shown that using equation (6.6) for the end images instead of (6.10) would produce artifacts in the solution. For image \( k = 1 \), assuming \( E(m^1) < E(m^2) \) and recalling (6.5), equation (6.6) in expanded form would be,

\[
\frac{dm^{(1)}}{d\xi} = \frac{1}{|m^2 - m^1|^2} \left( m^2 \times m^2 \times \nabla E |_{m^1} - m^1 \times m^2 \times \nabla E |_{m^1} \right. \\
\left. - m^2 \times m^1 \times \nabla E |_{m^1} - m^1 \times m^1 \times \nabla E |_{m^1} \right) + k_s |m^2 - m^1|^2 .
\]  

Assuming that convergence of the above equation of motion implies equilibration to a micromagnetic minimum, \( \frac{dm^1}{d\xi} = 0 \rightarrow m^1 \times \nabla_c E |_{m^1} = 0 \), the right hand side of equation (6.11) must also equal zero. However, there is no indication why this condition should be
met, even for $k_s = 0$. Moreover, since the first and second image are not expected to be overly similar, $\mathbf{m}^2 \times \nabla E|_{m^1} \neq 0$, and the condition is never met. Hence the evolution of the end images should only be performed according to equation (6.10).

In summary, freeing the end images in the NEBM allows for the relaxation of the initial and final state to the nearest energy minimum. The relaxation proceeds concurrently with the search for the MEP. The convenience of loose ends is that an independent simulation for obtaining the equilibrated initial and final states needed for the NEBM with fixed ends can be avoided, thus simplifying the overall procedure. A case when the fixed ends approach should be used instead of the loose ends approach is when the calculation of energy barriers between non-equilibrium states is sought.

Often times, in the loose ends approach, the relaxation of the initial and final states toward the local minimum proceeds faster than the convergence of equation (6.6) to the MEP. Therefore, it is reasonable to reduce the number of unknowns from $3Nn$ to $3N(n - 2)$ by excluding the degrees of freedom of the end images from the simulation once the end images have converged. This can be done on the fly by simply defining convergence criteria and monitoring the residual of the end images during the simulation. Following this procedure, the computational time can be decreased on the whole, which can be helpful for the case of large problem sizes and complex systems and energy landscapes.

6.2.4 Improving the Initial Guess Path

It has been observed that linear interpolation of end images for select problems can produce initial guess paths that lead the iterative path finding procedure astray. Using a guess path extracted from an LLG simulation, in which an applied field is used to drive the system from the initial to the final state, is often preferred, as so obtained a path is believed to more closely resemble the MEP. However, defining an applied field to take a system from one point in configuration space to another, can often be nontrivial or demanding. This is especially the case when complex metastable domain structures are involved. Exploring alternative strategies for specifying initial guess paths, which do not require user input, can be of great utility, not only for searching for the MEP between complex configurations, but also for automating and optimizing the path search for the case of simple problems.

Consider two arbitrary states defined by image vectors $\hat{\mathbf{m}}^0$ and $\hat{\mathbf{m}}^n$. We wish to
obtain images $m^k$ for $k \in [2, n - 1]$ in order to define the initial guess path for the NEBM. Such images may be obtained from a simulation of LLG dynamics in the high damping approximation, where a new field $H^s$ is artificially introduced to help strategically guide the transition from the initial to the final state. At an arbitrary node $i$, the new field is

$$H_i^s = -H_{i}^{\text{eff},\parallel} + \varepsilon^s \hat{m}_i^n. \quad (6.12)$$

Here, $H_{i}^{\text{eff},\parallel} = (H_{i}^{\text{eff}} \cdot \hat{m}_i^n)\hat{m}_i^n$ is the component of the physical micromagnetic effective field at node $i$ parallel to the direction of the magnetization unit vector at the final state $\hat{m}_i^n$, and $\varepsilon^s$ is a scaling parameter. The field $H^s$ will act on the instantaneous magnetization throughout the system so as to orient it along the final magnetization direction $m^n$. The value of the scaling parameter $\varepsilon^s$ is determined at each node and time step according to weight criteria which serve to ensure that the contribution from $H^s$ is marginal, so that the reconfiguration from the initial to the final state maximally reflects exchange, magnetostatics, magnetocrystalline anisotropy, and other physical interactions. Optimizing weight criteria to improve method performance is in development.

We note that for simple problems, when the initial and final states happen to be mutually antiparallel, i.e., $\hat{m}^0 \times \hat{m}^n = 0$, then $H^s = 0$. In such circumstances, perturbation or noise is introduced to initiate the transition process.

The performance of the automated method described here has been tested on
several standard examples. For the case of a single domain particle with uniaxial anisotropy, the method yields a guess path representing coherent rotation of magnetization for the transition between the two stable configurations. Such a guess path coincides with the MEP. We have also considered the common example of an elongated grain with the initial and final states shown in Fig. 6.3a. The obtained transition involves nucleation at both ends of the grain, followed by domain wall propagation toward the center. This is also the reversal mode obtained when a strong external field is applied in the absence of thermal agitation. To obtain an improved guess path, we introduce noise in the form of thermal fluctuations (section 5.2). Figure 6.3b shows the improved guess path thus obtained. The transition involves the nucleation and propagation of only one domain wall, and resembles the MEP very closely. Alternative revisions to the method for avoiding scenarios such as illustrated in Fig. 6.3a may include introducing tolerance driven sweep lines or expanding bubbles, exterior to which $H^s = 0$. Lastly, Fig. 6.4 shows an example of a guessed transition between two vortex states having opposite chirality and same polarity. Improvements to the method will involve developing improved criteria for the determination of $\varepsilon^s$ at each node and time step during integration of the LLG equation. The ultimate extent to which the described method can produce improved guess paths for different problem types remains to be determined.

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7 Modeling of Polycrystalline Films and Devices

The present chapter is devoted to the modeling of polycrystalline magnetic nanostructures and devices. The microstructure of granular films is described. Voronoi discretization is shown to properly resolve magnetization texture, in addition to optimally accounting for grain geometry, when the granular dimensions are below the exchange length [Lubarda et al., 2012a]. The effects of Voronoi tessellation and subgranular tetrahedral discretization on problem size and numerical stiffness are discussed. A procedure for the numerical patterning of granular systems, including nanowires and nanoislands, is outlined. The described modeling is the basis for simulation studies reported in chapters 9 and 10.

7.1 The Microstructure of Polycrystalline Magnetic Thin Films

Polycrystalline (granular) magnetic thin films are the basis for a number of current and emerging technologies, including perpendicular magnetic recording (PMR), heat assisted magnetic recording (HAMR), bit patterned media (BPM), and magnetic random access memory (MRAM). They are model systems for many recent experimental studies which include characterization studies, studies of reversal modes and domain wall propagation under the influence of fields and spin currents, as well as the investigation of current-tunable spin transfer torque (STT) oscillators for microwave generation. The microstructure of granular systems and the distribution of material and structural properties of the grains can significantly impact the performance of polycrystalline magnetic devices and affect the results of experimental studies. It is of great interest,
therefore, to micromagnetically model these systems to characterize them and investigate their performance over a wide range of parameter space.

The specific microstructure of a polycrystalline magnetic thin film is the result of a range of processes occurring during film growth. The majority of magnetic thin films used for applications outlined above are sputter deposited. Sputter deposition involves the bombardment of the target material with a beam of ions, typically Ar\(^+\), whereby target atoms are ejected from the host sample and deposited onto a substrate or seed layer. Initially, islands of the target species form on the substrate, interlocking with the substrate crystallographic direction. Once nucleated, the islands expand, eventually coalescing and forming grain boundaries. The final microstructure of the thin film depends on the energetics during nucleation, coalescence, and post-coalescence phases. The energetics of island formation depends on the substrate surface, target species, partial pressures, substrate temperature, deposition rate, and other deposition and postprocessing conditions. The grain boundaries change shape and move during grain growth in a way that minimizes surface and interfacial energies. As a result, grain boundaries tend to be rectangular in shape. If an oxide impurity is present in the film, it typically diffuses to the grain perimeter to decrease the total energy. In the case of magnetic recording media fabrication, oxide impurities are intentionally introduced to exchange decouple the ferromagnetic grains. The target and substrate are selected and the deposition conditions regulated such that the desired granular structure is obtained. Figure 7.1 shows an example of a magnetic recording medium with 8 nm average grain size (in the lateral
direction) and 1 nm wide oxide segregant separating the grains.

Despite the ability to control many of the conditions during the film growth and postprocessing phases, in the end, there always exists a distribution of structural and material properties of the grains. Of particular importance to the applications outlined at the beginning of this section are the distributions in grain size, surface and interface roughness, anisotropy energy density and easy axis direction, saturation magnetization, and damping constant. This chapter is dedicated to the micromagnetic modeling of complex granular systems which takes into account the wide variety of distributions and imperfections which characterize realistic devices.

7.2 Voronoi Discretization

7.2.1 Optimal Grain Representation

In chapter 3 we described modeling of magnetic bodies based on the linear basis finite element representation, where tetrahedral elements were used to discretize magnetic volumes. This approach was advantages for modeling complex geometries and bulk systems such as recording heads and read heads, patterned nanoparticles of arbitrary shape, nanowires and nanorings, multilayer spin valves, and extended films supporting spin waves, when the granular microstructure and material texture were chosen to be ignored. However, the listed structures and devices are by and large composed of granular magnetic thin films. When the effects of material and structural distributions of the grains on device performance (e.g., magnetization response to external fields, thermal fluctuations, or spin transfer torques) need to be studied, a more suitable discretization scheme than just finite element tetrahedral discretization is required that can fully resolve the granular microstructure of the system. Voronoi discretization is well suited for modeling granular systems due to the direct geometrical correspondence between a Voronoi cell and a crystallite. Voronoi representation of granular systems further allows each grain to be treated as a macrospin. This is especially valuable in the case of magnetic recording media modeling where grains are exchange decoupled, homogeneous, and of laterally coherent magnetization. When the magnetization within each grain must be resolved in more detail, tetrahedral or hexahedral discretization (section 3.1) can be performed subsequent to Voronoi tessellation. In the present section we provide an outline of Voronoi discretization and highlight its advantages in terms of computational
complexity and simulation time, as well as its convenience for modeling granular systems.

Since magnetic recording performance is critically dependent on the microstructure of the granular medium, we begin our discussion of Voronoi discretization with attention to granular recording media, and later generalize the discussion to a wider variety of granular magnetic structures and devices, such as nanowires, bit patterned media, and read heads.

In today’s magnetic recording media, the average grain diameter is roughly 7–8 nm. With a typical media saturation magnetization of $M_s \approx 700$ emu/cm$^3$, anisotropy energy density $K \approx 5$ Merg/cm$^3$, and exchange constant $A \approx 1.3$ erg/cm, the lateral grain size falls below the critical length scales characterizing magnetization texture defined by exchange lengths $l_{\text{ex}}^{\text{ms}} \approx \sqrt{A/(2\pi M_s^2)}$ and $l_{\text{ex}}^{\text{anis}} \approx \sqrt{A/K}$. As a result, the magnetization of each exchange decoupled grain can be considered laterally uniform. If the thickness of the grain is below these critical lengths, as well, the grain as a whole can be expected to behave as a single domain particle, and can be modeled as such (Fig. 7.2a). Conversely, if the grain thickness is greater than these critical lengths, the grain can be vertically discretized until the condition is met (Fig. 7.2b). This leads to the least number of discretization elements needed to resolve the magnetization dynamics and grain geometry, simultaneously.
7.2.2 Comparison between Voronoi Discretization and Other Discretization Schemes

Other discretization techniques used in modeling granular systems are the finite differences method (FDM) and finite element method (FEM) based on tetrahedral discretization. These methods have several disadvantages. FDM is not able to adequately account for the microstructure of granular systems because finite differences discretization is based on rectangular prisms. In addition to inaccurate representation of the granular system geometry, FDM may produce artifacts in the recorded pattern and signal-to-noise ratio (SNR) of magnetic recording media that can be traced back to the periodicity produced by the finite differences discretization scheme.

FEM does not encounter this problem because it correctly takes into account the granular system microstructure (as long as grain volumes are predefined, e.g., by using Voronoi tesselation beforehand) owing to a discretization based on tetrahedral elements which can accurately represent grain geometry. However, for perpendicular magnetic recording media, heat assisted magnetic recording media, and bit patterned media, the grains are around 10 nm in diameter or smaller, and behave as single domain particles. Hence, the finite element representation for many granular magnetic systems results in an overdiscritization, producing an unnecessarily large number of unknowns (over an order of magnitude greater than needed), which substantially increases the time required to simulate magnetization dynamics. Additionally, in case of granular systems with reduced intergranular coupling (a nonstiff system), the superfluous discretization of each grain generates a numerically stiff problem (section 8.2), which additionally slows simulations.

In comparison with finite differences, the finite element method has another disadvantage that limits computational speed: the irregularity of the FEM mesh does not permit the fast Fourier transform (FFT) to be used in the evaluation of the magnetostatic field, as conventionally done with FDM to reduce the number of computational operations from $O(N^2)$ to $O(N \log N)$.

In the following sections we describe micromagnetic modeling of granular magnetic structures based on numerical methods which combine the benefits and avoid the shortcomings of FDM and FEM. Each grain is represented by a Voronoi cell, which is treated as a single domain particle (macrospin), thereby keeping the number of unknowns to a minimum, while fully accounting for the microstructure of the granular system. For cases when the single domain approximation fails, tetrahedral or hexahedral discretization
in conjunction with Voronoi tessellation is used. A nonuniform fast Fourier transform (NUFFT) method is employed for the computation of magnetostatic interactions (section 8.1.2). The code is implemented on massively parallel graphics processing units (GPUs; section 8.3). The capability of the developed code to address a variety of problems is discussed. This includes characterization and recording on conventional and bit patterned media, operation of spin-valves and magnetic tunnel junctions (MTJs) used for MRAM and read heads, domain wall propagation in nanowires, and spin torque nanooscillators.

### 7.3 Granular System Modeling

In order to construct a model of a granular system, whether a single polycrystalline film, or a more complex patterned multilayered structure, a procedure resembling actual fabrication is followed. The sequence of steps summarized in chronological order is: seed layer nucleation, granular segregation (in case of exchange decoupling), film growth,
nucleation of new layers (in case of multilayer modeling), and postprocessing (e.g., patterning). Nucleation of the seed layer begins with a user-specified distribution of coplanar seed points which are given as input to a two-dimensional Voronoi tessellator. The tessellator in turn generates a two-dimensional mosaic of Voronoi cells (Fig. 7.3a) and provides information regarding the connectivity between the cells. Using centroids of thus generated Voronoi cells as seed points for a subsequent tessellation improves the quality of the Voronoi diagram to better reflect realistic media. Subsequent to this, the cells may be separated from each other by a controllable margin (Fig. 7.3b), to reflect the result of the actual segregation process. Extrusion of the two-dimensional cells in the vertical direction mimics columnar layer growth. Additional layers may be “grown” for a multilayer structure. Distributions in grain size, columnarity of the grains, intergranular separation, and interface roughness can be controlled during the construction process based on user-specified input.

Figure 7.3c shows a general multilayer structure consisting of three magnetic layers and two nonmagnetic interlayers, each having different properties and layer thicknesses. The different magnetic layers are seen to consist of two, three, or four sublayers (see insert to Fig. 7.3). An arbitrary number of sublayers can be assigned to each layer to provide the additional discretization required in the vertical direction. This feature is especially important for the case of domain wall-assisted reversal (section 9.1.4) or appreciable head field gradients in the vertical direction. Figure 7.3d shows the surface roughness and distribution of intergranular separation that can be induced at different stages during the numerical growth process. Material parameters are chosen to be constant within a single grain, but vary from grain to grain. The distributions and material properties such as the distributions in easy axis direction, anisotropy, saturation magnetization, and damping can be specified as Gaussian or lognormal with an associated mean and standard deviation. If necessary, distributions within a given grain can also be specified by performing additional discretization in the vertical and lateral directions. The granular film may also be patterned into nanowires, BPM, or any arbitrary shape using a three-dimensional numerical stencil mask to exclude cells that do not fall within the masked region and to modify the grain geometry at the mask perimeter (section 7.4).
Figure 7.4: Numerically pattered granular systems: (a) Granular frusta with and without subgranular tetrahedral discretization; (b) notched granular nanowire with and without subgranular tetrahedral discretization; (c) array of granular nanoislands.

7.4 Numerical Stenciling for Bit Patterned Media, Nanowires, and Devices

An accurate representation of polycrystallinity at the nanoscale is not only important for modeling granular films, such as continuous recording media, but is also essential for faithfully capturing the fine details of the nanostructure of bit patterned media, nanowires, and other devices which are manufactured from granular thin films by patterning techniques. In analogy with the fabrication process of such structures, our modeling procedure begins with the development of the continuous granular thin film model (section 7.3), proceeds with the application of a numerical stencil mask which defines the region(s) of the film we wish to preserve or obliterate, and concludes with the prescribed modifications to the film geometry.

The numerical stencil mask used for patterning may be defined in several ways. The most common definitions are expressed in terms of geometrical objects, such as circles or polygons, which define the mask contour. Lattices may also be specified, to define sites at which the geometrical objects are to be placed. This feature allows efficient modeling of BPM and MRAM elements.

The two-dimensional geometrical objects which define the mask contour may be specified differently at different stages of the numerical patterning process, and the patterning depth at each stage may be independently controlled, allowing for a multiphase patterning procedure and the modeling of highly complex systems and devices. Further modeling capability is achieved by allowing the geometrical objects (masks) to be three-
dimensional, to include ellipsoids or frusta, as well as allowing for different lattices types (rectangular, hexagonal, rhombic, etc.). Another feature is the possibility to controllably introduce irregularities (or nonuniformities), both in the locations of the lattice sites, and in the mask shapes. This is done by associating a standard deviation with the lattice spacing(s) or the geometric variable(s) defining the mask type (e.g., diameter, in the case of a circle). The flexibility to specify irregularities is particularly important for the analysis of SNR in BPM.

Once the numerical stencil is completely defined, numerical patterning of the granular film model may begin. The process proceeds according to the algorithm by which Voronoi cells outside of the mask(s) are removed, and cells at the mask perimeter conformingly modified. A mask may be alternatively specified as “negative”, in which case interior cells are dispelled, while exterior cells are preserved. The possibility of assigning a polarity to a mask is useful in the case of multiphase patterning for the construction of complex geometries.

We note that during the numerical patterning process, significant care has to be taken to appropriately update the cell coupling information, such as nearest neighbor arrays and interface coupling areas (important for exchange interactions), as the removal and tailoring of cells results in new cell identification numbers and modified connectivity. Alternatively, a sorting algorithm may be used to identify neighboring cells and to detail coupling information from scratch.

Once the granular film model is numerically patterned into the desired structure and the coupling information has been updated, the new model may be submitted for simulation (see Fig. 7.4 for examples of patterned granular systems). In case of a simulation in which the Voronoi cells are to be treated as single domain particles, tensors may be computed for near-field interactions, and the magnetization dynamics can be traced following the description given in section 7.5. Alternatively, the cells of the patterned model may be sub-discretized with tetrahedrons (chapter 3.1) or hexahedrons [Chang et al., 2012a] using meshing software such as Cubit or GID (Fig.7.4), and simulated according to [Chang et al., 2011] and the description provided in chapters 3–5.
7.5 Calculation of Micromagnetic Fields in Granular Systems Discretized by Voronoi Cells

The micromagnetic simulation of granular systems described above requires the integration of the Landau-Lifshitz-Gilbert (LLG) equation, or one of its extensions that may include STT terms, thermal fields, etc. The standard LLG equation in discretized form gives an expression for the torque acting on each cell $i$ as

$$\frac{d\hat{m}_i}{dt} = -\frac{\gamma}{1 + \alpha_i^2} \left[ \hat{m}_i \times \mathbf{H}_{\text{eff}}^i + \alpha_i \hat{m}_i \times (\hat{m}_i \times \mathbf{H}_{\text{eff}}^i) \right],$$  \hspace{1cm} (7.1)

where $\hat{m}_i$ is the instantaneous unit vector in the direction of the cell’s magnetic moment, $\alpha_i$ and $\gamma$ represent the damping and gyromagnetic ratio, and $t$ is the time. The effective field on each cell $i$ can be represented as the sum of the Zeeman, anisotropy, exchange, and magnetostatic fields, $\mathbf{H}_{\text{eff}}^i = \mathbf{H}_{\text{Zee}}^i + \mathbf{H}_{\text{anis}}^i + \mathbf{H}_{\text{ex}}^i + \mathbf{H}_{\text{ms}}^i$.

7.5.1 Zeeman Field

The Zeeman field is the applied field specified as input in the form of an analytical expression, or a data file from which the field values at the cell centroids can be interpolated. For cell $i$, this can be expressed as

$$\mathbf{H}_{\text{Zee}}^i = \mathbf{H}_a(\mathbf{r}_i),$$  \hspace{1cm} (7.2)

where $\mathbf{r}_i$ is the position vector pointing to the cell centroid. The Zeeman field can represent the uniform external field that is swept during an MH-loop measurement, or it can represent the field produced by a write head used for magnetic recording. A recording field profile can be obtained from a separate simulation of a write head, such as discussed in [Escobar et al., 2012b], and used as input to the Voronoi solver. This is done for simulations presented in sections 9.2 and 10.4.

In case of strong gradients and large cell sizes, averaging of the applied field over the cell surface or volume can be used to improve accuracy. If higher accuracy is required, the cells can be further discretized in both vertical and lateral directions (section 7.4).

7.5.2 Magnetocrystalline Anisotropy Field

The expression for the uniaxial magnetocrystalline anisotropy field (section 2.2.4) on cell $i$ is

$$\mathbf{H}_{\text{anis}}^i = \frac{2K_i}{M_{s,i}} \left( \hat{m}_i \cdot \hat{k}_i \right) \hat{k}_i,$$  \hspace{1cm} (7.3)
For $K_1 > 0$, the energy minima are obtained when the magnetization is along one of the four $\langle 111 \rangle$ directions (two orientations possible for each direction). For $K_1 < 0$, these eight possibilities correspond to energy maxima, and the three $\langle 100 \rangle$ directions correspond to the energy minima.

where $K_i$, $\hat{k}_i$, and $M_{s,i}$ are the magnetocrystalline anisotropy energy density, easy-axis direction, and saturation magnetization. For cubic crystals such as nickel or iron, the magnetocrystalline field can be derived from the differentiation of the cubic anisotropy energy density with respect to the magnetization. Cubic anisotropy energy density can be written as

$$
\varepsilon_{\text{anis}} = K_0 + K_1 \left( m_1^2 m_2 + m_2^2 m_3^2 + m_3 m_1^2 \right) + K_2 m_1^2 m_2^2 m_3^2, \quad (7.4)
$$

where $m_1 = \hat{m} \cdot \hat{k}_1$, $m_2 = \hat{m} \cdot \hat{k}_2$, and $m_3 = \hat{m} \cdot \hat{k}_3$, and $\hat{k}_1$, $\hat{k}_2$, and $\hat{k}_3$ represent the $[100]$, $[110]$, and $[001]$ crystallographic directions. For iron, near room temperature, $K_1 = 4.8 \times 10^5 \text{erg/cm}^3$ and $K_2 = -1.0 \times 10^5 \text{erg/cm}^3$, and the energy minima are obtained when the magnetization is along one of the four $\langle 111 \rangle$ directions (two orientations possible for each direction). For nickel at about room temperature, $K_1 = -4.5 \times 10^4 \text{erg/cm}^3$ and $K_2 = -2.3 \times 10^4 \text{erg/cm}^3$, and these eight possibilities correspond to energy maxima (Fig. 7.5). The cubic anisotropy field for cell $i$ is derived as (section 2.2)

$$
H_{i,\text{anis}} = -\frac{1}{M_{s,i}} \frac{\delta \varepsilon_{\text{anis}}}{\delta \hat{m}_i} = -\frac{1}{M_{s,i}} \left( \begin{array}{c}
2K_{1,i} \left( m_{1,i} m_{2,i}^2 + m_{3,i}^2 m_{1,i} \right) + 2K_{2,i} m_{1,i} m_{2,i}^2 m_{3,i}^2 \\
2K_{1,i} \left( m_{1,i}^2 m_{2,i} + m_{2,i} m_{3,i}^2 \right) + 2K_{2,i} m_{1,i}^2 m_{2,i} m_{3,i}^2 \\
2K_{1,i} \left( m_{2,i}^2 m_{3,i} + m_{3,i} m_{1,i}^2 \right) + 2K_{2,i} m_{1,i} m_{2,i}^2 m_{3,i}^2
\end{array} \right). \quad (7.5)
$$
Surface anisotropy fields can be derived from the expression

$$
\mathbf{H}_i^{s,\text{anis}} = -\frac{1}{M_{s,i}t_i} \frac{\delta \varepsilon_i^{s,\text{anis}}}{\delta \mathbf{m}_i},
$$

where

$$
t_i = \frac{S_i}{V_i},
$$

and $S_i$ is the area of the cell surface characterized by surface anisotropy energy density $\varepsilon_i^{s,\text{anis}}$, and $V_i$ is the cell volume. In our derivation we assumed a constant magnetization and energy density within each cell, consistent with the Voronoi discretization model, as described.

The volume of the cell appearing in (7.7) can be calculated as the base area of the cell multiplied by the cell thickness. However, a more general expression is needed for irregular cell shapes such as those illustrated in Fig. 7.6a. An analytical expression can be obtained exploiting Gauss’s divergence theorem, which states that for any surface
$S$ enclosing volume $V$ and having $\hat{n}$ as its outward unit normal,

$$\int_V \nabla \cdot \mathbf{A} \, dV = \int_S \mathbf{A} \cdot \hat{n} \, dS,$$

(7.8)

where $\mathbf{A}$ is an arbitrary vector field. If we chose $S$ (and hence $V$) to represent our arbitrary cell geometry, and choose $\mathbf{A} = \frac{1}{3}\mathbf{r} = \frac{1}{3}(x\hat{x} + y\hat{y} + z\hat{z})$, so that $\nabla \cdot \mathbf{A} = 1$, we have, from equation (7.8),

$$V = \frac{1}{3} \int_S \mathbf{r} \cdot \hat{n} \, dS.$$

(7.9)

This can be decomposed into a sum of integrals over all triangles $t$ which comprise the triangulated cell boundary surface (Fig. 7.6b),

$$V = \frac{1}{3} \sum_t \int_{S_t} \mathbf{r}_t \cdot \hat{n}_t \, dS_t.$$

(7.10)

The dot product $\mathbf{r} \cdot \hat{n}_t$ represents the projection of the position vector onto the triangle outward unit normal. Since the position vector $\mathbf{r}$ is constrained to the triangle plane, the projection is identical for any such $\mathbf{r}$. Hence, the expression for the volume of a triangulated cell of arbitrary geometry simply reduces to

$$V = \frac{1}{3} \sum_t \left( \mathbf{r}_{t\text{arb}} \cdot \hat{n}_t \right) S_t,$$

(7.11)

where $\mathbf{r}_{t\text{arb}}$ is a position vector of an arbitrary point belonging to triangle $t$, and $S_t$ is the triangle area. A convenient choice for $\mathbf{r}_{t\text{arb}}$ is the position vector pointing to one of the vertices of triangle $t$. The volume of the cell, derived here, will also be used in the computation of the micromagnetic fields in the subsequent sections.

### 7.5.3 Exchange Fields

In the Voronoi discretization scheme, each cell represents a single domain (macrospin) particle. When cell $i$ is exchange coupled to cell $j$ across an interface, it is most natural that the strength of the exchange coupling be defined through the interface energy density $J_{ij}^{ex}$ (erg/cm$^2$). The exchange energy of a system of two bilinearly exchange coupled cells (section 2.1.7) with unit moment vectors $\hat{\mathbf{m}}_i$ and $\hat{\mathbf{m}}_j$ is

$$E_{ij}^{ex} = -\int J_{ij}^{ex} \hat{\mathbf{m}}_i \cdot \hat{\mathbf{m}}_j \, dS,$$

(7.12)

which, owing to the homogeneous macrospin representation of the cells, reduces to

$$E_{ij}^{ex} = -J_{ij}^{ex} S_{ij} \hat{\mathbf{m}}_i \cdot \hat{\mathbf{m}}_j,$$

(7.13)
where $S_{ij}$ is the area of the interface between the two cells. The assumption of constant interfacial energy density $J_{ij}^{\text{ex}}$ in the macrospin Voronoi representation (7.13) is to no loss of generality, since one can always write $\int J_{ij}^{\text{ex}}(r) \, dS$ as $\left\langle J_{ij}^{\text{ex}} \right\rangle S_{ij}$. The contribution to the exchange field on cell $i$ due to cell $j$ can now be written as

$$H_{ij}^{\text{ex}} = -\frac{1}{M_{s,i}V_i} \frac{\delta E_{ij}}{\delta \hat{m}_i} = \frac{S_{ij}J_{ij}^{\text{ex}}}{M_{s,i}V_i} \hat{m}_j.$$  \hspace{1cm} (7.14)

More generally, the total exchange field on cell $i$ due to all nearest neighbor cells $j$ with which $i$ is exchange coupled is

$$H_i^{\text{ex}} = \sum_{j \in \text{n.n.}} S_{ij}J_{ij}^{\text{ex}} \frac{1}{V_i M_{s,i}} \hat{m}_j.$$  \hspace{1cm} (7.15)

Though equation (7.15) provides a general expression for the net exchange field on cell $i$, it remains important to distinguish between three physically distinct exchange contributions: intra-granular exchange, inter-granular exchange, and inter-layer exchange.

**Intragranular Exchange**

Intragranular exchange is the exchange interaction occurring between spins within a single grain. The strength of this interaction depends on the exchange stiffness constant $A_{\text{ex}}$ (erg/cm) of the grain material. In the Voronoi representation, each grain is represented by a single Voronoi cell, or a vertical stack of Voronoi cells. If the grain is expected to behave as a single domain particle, a single cell is used to model the grain, and intragranular exchange need not be considered. When a stack of cells is used to represent the grain, then the interfacial exchange energy density $J_{\text{ex}}^{\text{ij}}$ between two adjacent cells in the uniformly partitioned stack is given by $2A_{\text{ex}}/t$, where $t$ is the thickness of each cell in the grain. The intergranular contribution to the exchange field can be determined from (7.15).

**Intergranular Exchange**

Intergranular exchange is the exchange interaction between the laterally adjacent cells of the same layer, which, in the case of magnetic recording media, are weakly coupled across an oxide barrier. The strength of coupling is most naturally defined through the intergranular (interface) energy density $J_{ij}^{\text{ex}}$ (erg/cm$^2$). However, in characterization measurements of magnetic recording media, the effective stiffness constant $A_{\text{ex}}$ (erg/cm) is usually a more convenient parameter to work with. If the average grain diameter is
\[ J_{\text{ex}} = \frac{2A_{\text{ex}}}{\Delta}, \]

and equation (7.15) can again be used to compute the intergranular contribution to the exchange field.

**Interlayer Exchange**

Interlayer exchange is the exchange interaction between grains separated by a nonmagnetic spacer layer. The strength of this interaction is defined by the interlayer energy density \( J_{\text{ex}} \) (erg/cm\(^2\)). Interlayer coupling may be ferromagnetic \( (J_{\text{ex}} > 0) \) or antiferromagnetic \( (J_{\text{ex}} < 0) \). The interlayer exchange field between two vertically adjacent cells belonging to different layers is again given by equation (7.15). For the case of biquadratic coupling (section 2.1.7), with interfacial energy density defined as \( \varepsilon_{\text{ex}}^{\text{bq}} = J_{\text{ex}}^{\text{bq}} \left( \hat{m}_+ \cdot \hat{m}_- \right)^2 \), the associated field on cell \( i \) due to cell \( j \) can be expressed as

\[
H_{\text{ex,bq}}^{ij} = -\frac{S_{ij}}{M_{s,j}V_i} \delta \varepsilon_{ij}^{\text{ex,bq}} = -\frac{2S_{ij}J_{\text{ex,bq}}^{\text{ex,bq}}}{M_{s,j}V_i} (\hat{m}_i \cdot \hat{m}_j) \hat{m}_j, \tag{7.16}
\]

where \( S_{ij} \) is the area of the coupling interface between cell \( i \) and \( j \), \( V_i \) is the volume of cell \( i \), and \( J_{\text{ex,bq}}^{\text{ex,bq}} \) (erg/cm\(^2\)) quantifies the strength of biquadratic coupling between the two cells.

**7.5.4 Magnetostatic Field**

The evaluation of the magnetostatic contribution to the effective field is most involved, and proceeds in several steps. First, a specialized algorithm (Fig. 7.6c) identifies all cells \( j \) that fall within a critical distance of cell \( i \). If two cells are sufficiently far apart, the dipolar approximation can be used to compute the magnetostatic interaction with high accuracy. The magnetostatic field on cell \( i \) due to cell \( j \) in the dipolar approximation reads

\[
H_{\text{ms}}^{ij} = \frac{3r_{ij} \left( \mu_j \cdot r_{ij} \right)}{|r_{ij}|^5} - \frac{\mu_j}{|r_{ij}|^3}, \tag{7.17}
\]

where \( r_{ij} \) is the position vector extending from the centroid of cell \( j \) to the centroid of cell \( i \), and \( \mu_j \) is the magnetic moment of cell \( j \), which, in terms of saturation magnetization and cell volume, is expressed as \( \mu_j = M_{s,j}V_j \hat{m}_j \). Conversely, for two proximal cells, where the dipolar approximation produces intolerable error, a tensor approach for the computation of the magnetostatic field is implemented, which fully takes into account the geometry of the particles. Within this approach, the magnetostatic field on cell \( i \) due
to cell $j$ is computed as
\[
H_{ij}^{\text{ms}} = N_{ij} \cdot M_j ,
\] (7.18)
where $M_j = M_{s,j} \hat{m}_j$ is the magnetization of cell $j$, and $N_{ij}$ is the demagnetization tensor, given by [Newell et al., 1993]
\[
N_{ij} = \frac{1}{V_i} \int_{S_i} \int_{S_j} \frac{dS_i}{|r_i - r_j|} .
\] (7.19)

Here, $dS_i = dS_i \hat{n}_i$, with $\hat{n}_i$ as the outward unit normal to the surface $S_i$, and $V_i$ is the volume of cell $i$. The above expression is an integration over the surfaces of the two cells, through which full information regarding cell shapes is included. The inner integral in equation (7.19) can be evaluated using analytical expressions, while the outer integral is computed using quadrature rules [Chang et al., 2011,Peterson et al., 1998]. Finally, we note that (7.19) is also valid when self-interaction is considered, i.e., $i = j$.

Since the magnetostatic interaction is a far field interaction whose evaluation typically involves $O(N^2)$ operations, advanced techniques are necessary to boost computational speed and reduce memory costs to allow simulations of exceedingly large problems. An outline of three acceleration techniques, the nonuniform fast Fourier transform (NUFFT) method, the nonuniform grid (NG) method, and portation to massively parallel graphics processing units (GPUs) can be found in chapter 8.

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8 Acceleration Schemes for Micromagnetic Solvers

The micromagnetic tools developed in chapters 3–7 for the computation of fields, currents and torques must be complemented with powerful acceleration techniques to allow for practical simulations of micron-sized devices and finely discretized systems. This chapter provides an outline of the acceleration schemes that have enabled the large-scale simulation studies presented in part III of this dissertation.

8.1 Computation of Far Field Interactions

The speed of a micromagnetic simulator and its ability to handle large problem sizes is greatly determined by the methods it employs for the computation of far field interactions. In micromagnetics, the central far field interaction is the magnetostatic interaction, which, in a discretized model, involves $M$ sources and $N$ observers. In many cases the sources and observers are one, implicating $O(N^2)$ computational complexity for direct evaluation algorithms. Another important far field interaction is that between current-induced magnetic fields and the magnetization. When an electric current is controlled externally, say through a voltage bias, the induced magnetic field is called the Oersted field (or Amperian field) (sections 4.2.2). As the Oersted field extends across all space, its direct computation involves $O(N^2)$ arithmetic operations. Similarly, the evaluation of eddy-current fields, once the eddy currents are known, requires $O(N^2)$ operations. For the computation of eddy currents, see [Hrkac, 2011, Chang et al., 2013].

The $O(N^2)$ complexity implicit to direct far field evaluation renders simulations based on direct methods unpracticable for problems involving many degrees of freedom, due to exorbitant memory requirements and excessive computation time. A number
of alternative methods with asymptotic complexity $O(N \log N)$ and $O(N)$ have been developed to replace direct methods for far field calculations. For the case of finite differences modeling, where regular hexahedral elements (cubes or rectangular prisms) are used in discretization, the fast Fourier transform (FFT) method can be used to reduce operational complexity of far field evaluation to $O(N \log N)$, provided that overall periodicity conditions are met, for which a zero-padding technique exists.

Though powerful for finite-differences modeling, the FFT method is inapplicable to modeling based on tetrahedral (section 3.1) or Voronoi (section 7.2) discretization, or any other discretization technique characterized by irregularity or nonuniformity of the mesh. Fortunately, a number of reduced complexity methods for far field evaluation have been developed for the case of irregularly distributed sources/observers. These methods rely on hierarchical schemes, compression techniques, and/or multigrid representations. The fast multiple method (FMM) is an example of a hierarchical method that is $O(N)$ asymptotically complex. However, a method should not be solely judged based on asymptotic order, as performance can be geometry-sensitive and overhead expenses in certain cases may run high. Due to overhead costs per field evaluation for a smaller/moderate problem size $N$, the overall number of performed operations can in fact be greater for an $O(N)$ method than for an $O(N \log N)$ method.

In the subsequent two sections, we provide a synopsis of the $O(N)$ nonuniform grid (NG) interpolation method and the $O(N \log N)$ nonuniform FFT method (NUFFT), as developed and implemented by S. Li et al. [Li et al., 2010, Li et al., 2012], and as used for the far field evaluation in micromagnetic simulations presented in part III of the present dissertation.

### 8.1.1 The Nonuniform Grid (NG) Interpolation Method

The nonuniform grid (NG) interpolation method is a hierarchical method based on a multilevel multigrid scheme, which capitalizes on the slow variation of the fields far from their sources to achieve an $O(N)$ asymptotic complexity. The method was introduced to micromagnetics by S. Li et al. for the evaluation of the magnetostatic, Oersted, and eddy fields. In addition to facilitating fast computation of all-to-all interactions, the reduced complexity algorithm greatly lowers memory consumption, thus enabling the simulation of problems of record size. The NG method is of great value not only in micromagnetics, but also electromagnetics, celestial mechanics, and other fields of study where long range
Interactions must be accounted for. The present section provides a brief outline of the algorithm, the implementation of which is described in [Li et al., 2010].

Consider an arbitrary body discretized into finite elements so that the consideration of magnetostatic interactions (or interactions with Oersted fields) involves $N$ effective magnetic charges (or current filaments) confined to the mesh nodes, as depicted in Fig. 8.1. In this example, the sources and observers are one, though the NG method is also applicable to problems where the observation and source domains are separate. In the preprocessing stage of the NG algorithm, the entire source domain is enclosed in a box, which is subsequently subdivided into eight smaller boxes. The larger box is referred to as the parent box, and the eight smaller boxes are called child boxes. Each of the eight child boxes are then subdivided into eight grandchild boxes, and each of these into eight great-grandchild boxes, and so on, until the average number of sources per box at the bottom of the ancestral (octal) tree falls within some predefined margin of optimality, at which point multilevel domain decomposition of sources is complete.
As can be seen from Fig. 8.1, some boxes may not include any sources. Such boxes may be discarded. This is largely the reason why the NG algorithm is highly suitable for systems of reduced dimensionality, such as thin-films, nanowires, and bit patterned media, where much of the space is unoccupied.

Once domain decomposition is complete and empty boxes discarded, sparse spherical nonuniform grids are constructed for boxes at all levels (Fig. 8.1). The grid points are distributed only as needed, with a sparsity that grows with increasing separation from the source. The nonuniform grid for each source box serves to sample the resultant field in the region of space occupied by distant observers. Cartesian grids are then constructed for observer boxes at all levels (in this example source boxes and observer boxes are one and the same).

With the nonuniform spherical and Cartesian multilevel grids in place, preprocessing is complete, and the evaluation of the far field at each simulation time step may proceed according to the following algorithm. First, for each box at the smallest-box level the fields due to sources enclosed by that box are evaluated by a direct method at all points belonging to the nonuniform grid associated with that particular box. After this, the fields at points belonging to the parent grids are interpolated from the field values at points distributed on the associated child grids, which hierarchically leads to the determination of the field at all the nonuniform grid points across all levels. In the third step of the algorithm, the values of the field at CG points at the largest-box level are interpolated from the field values at NG points at the equivalent box level. Values of the fields at the points belonging to the Cartesian grids associated with the child boxes are than interpolated from the known values at CG points of the parent boxes, sequentially yielding the far field across the coarsest (smallest box level) Cartesian grids. In the final step, the far field at all observer points (mesh nodes) is obtained via interpolation from the coarsest Cartesian grids. At this stage, the contribution of the near field, directly computed at each given node from sources in the source and nearest neighbor boxes, is added to the total potential. The hierarchical scheme implementing local interpolation results in $O(N)$ asymptotical complexity.

The ultimate performance of the NG method is critically dependent on the details of its implementation, such as the way the spherical nonuniform and Cartesian grids are constructed, the manner in which sparsity is regulated and grid points distributed, and the means by which interpolation is performed at different stages of the algorithm.
Memory management and transfer are another core consideration in the implementation of the NG method which can dramatically impact execution efficiency and capability to handle large problem sizes. A key feature of the NG code developed by S. Li et al., and used for the evaluation of far fields in many of the simulations presented in part III, is its implementation and high-level optimization for execution on massively parallel graphics processing unit (GPU) architectures, which provide great advantages over conventional central processing units (CPUs); section 8.3. A more elaborate account of the NG method with details of its implementation can be found in [Li et al., 2010, Li, 2012].

8.1.2 Nonuniform Fast Fourier Transform (NUFFT)

Reduced complexity methods used for the evaluation of far fields have a performance that typically varies with the problem size, model geometry, and frequency response. Hence, it is preferable to have more than one reduced complexity method available for the simulation of diverse systems and phenomena. Here, we provide a basic outline of the nonuniform fast Fourier transform (NUFFT) method, as developed and implemented by S. Li et al. [Li et al., 2012], which is used for many simulations presented in part III of the present dissertation.

The utility of the FFT method in the computation of far field interactions for the case of a uniformly and regularly discretized model has already been underscored in the introduction to section 8.1. The NUFFT method is an extension of the FFT method whose applicability extends to problems for which the discretization scheme employed yields a nonuniform/irregular mesh (e.g., tetrahedral, hexahedral, or Voronoi).

The procedure for calculating far fields using NUFFT goes as follows. First, the entire model is enclosed in a cube, which is uniformly divided into $N_{\text{box}}$ cubical boxes, as illustrated in Fig. 8.2. Each box contains a certain number of mesh nodes. The nodes represent sources of the far field, and simultaneously observers (in our case). To compute the far field at each mesh node, the sources are first projected onto the nodes of the box grid using interpolation methods. The problem reduces to a regular distribution of sources/observers, for which the FFT method is employed to compute the far field at each box-grid node. As the number of boxes $N_{\text{box}}$ is typically chosen for large problem sizes to be comparable to the number of mesh nodes $N$, the arithmetic complexity scales as $O(N \log N)$.

Once the field values at the box-grid nodes are obtained, they are used to
interpolate the values of the far field back onto the original observers (mesh nodes). Since the projection scheme misrepresents near field interactions, a correction must be made to ensure accuracy of result. Different approaches may be taken. The algorithm of S. Li et al. corrects for the near field interactions by subtracting the near field contribution calculated by the projection method, and by directly computing the near field contribution on each node of every box via a direct $O(n_i^2)$ method, where $n_i$ denotes the number of nodes included in the computation of the near field for observers within box $i$.

While the NUFFT method achieves $O(N \log N)$ asymptotical complexity, the overall performance, as for the case of the NG method (section 8.1.1), closely depends on the details of implementation of the various parts of the algorithm, including the projection algorithm and the employed interpolation schemes, the implementation of the conventional FFT, as well as the exact procedure for near field subtraction and correction. Memory handling and transfer between the different parts of the algorithm is another key determinant of overall NUFFT efficiency. This can be appreciated in the sophisticated NUFFT implementation of S. Li et al., where each step has been finely optimized, and the algorithm uniquely developed to maximally exploit the advantages of the graphics processing unit (GPU) architecture (section 8.3) on which it runs. More details of the NUFFT GPU algorithm and its implementation can be found in [Li et al., 2012, Li, 2012].
8.2 Numerical Integration Techniques

The efficiency of the evaluation of fields, currents, and torques, discussed in the previous sections, is not the sole determinant of overall simulator performance. A key role belongs to the numerical integration scheme, which determines the number of time steps (or field, current, and torque evaluations) required to achieve an accurate representation of the magnetization vector through time. In a word, the field, current, and torque evaluation efficiency determines the simulation time per time step, while the efficiency of the numerical integration scheme determines the number of time steps per simulated time.

The number of available numerical integration recipes for the simulation of physical processes is large. Applicability analysis narrows the selection of effective numerical integration algorithms for use in micromagnetics. Micromagnetic simulations presented in part III of this dissertation have largely been based on linear multistep methods (LMMs). The family of methods affords efficient solutions for both stiff and nonstiff systems. A problem is characterized as numerically stiff if the solutions produced by the explicit time integration routines demonstrate unwillingness to converge in spite of reducing the time step. Micromagnetic problems, where exchange interactions are a determining factor, produce a stiff system. Poor quality meshes with highly nonuniform discretization and small elements typically increase stiffness. Certain systems of interest are inherently nonstiff. An example of a nonstiff system is a granular exchange decoupled medium where each grain is regarded as a single domain particle (section 7.2.1).

In the coming sections, subsequent to reviewing LMMs, we present the implicit midpoint formula which can be used as a geometric integrator. Then, we review the Jacobian-free Newton-Krylov methods for the effective solution of nonlinear systems of equations produced by the implicit numerical integration schemes.

8.2.1 Linear Multistep Methods

To solve for the magnetization dynamics of a system out of equilibrium, the Landau-Lifshitz-Gilbert equation (2.4), or one of its extensions, must be integrated in time. The equation of motion can be generally expressed as

\[ \dot{\mathbf{m}} = \mathbf{\tau}(\mathbf{m}, t), \]  

(8.1)
where $\tau$ is the net torque on the magnetization due to the effective field, spin currents, damping, etc. We shall confine our attention to Eq. (8.1), but remark that much of the subsequent discussion may be extended to differential algebraic equations to include the dynamic equation in Gilbert (implicit) form, i.e., $\dot{m} = \tau(m, \dot{m}, t)$ (e.g., (4.19)).

In our modeling we assume the system to be discretized into finite elements. Equation (8.1) is to be understood as a system of coupled ordinary differential equations (ODEs), where

$$m = [ m_{1,x} \ m_{1,y} \ m_{1,z} \ m_{2,x} \ m_{2,y} \ m_{2,z} \ \ldots \ m_{N,x} \ m_{N,y} \ m_{N,z} ], \quad (8.2)$$

and

$$\tau(m, t) = [ \tau_{1,x}(m, t) \ \tau_{1,y}(m, t) \ \tau_{1,z}(m, t) \ \tau_{2,x}(m, t) \ \tau_{2,y}(m, t) \ \tau_{2,z}(m, t) \ \ldots \ \tau_{N,x}(m, t) \ \tau_{N,y}(m, t) \ \tau_{N,z}(m, t) ]. \quad (8.3)$$

The number of mesh nodes is $N$, and subscripts $x$, $y$ and $z$ indicate the three spatial components.

We discuss the numerical integration of the equation of motion (8.1) using LMMs. The general formula for a linear multistep method for the ODE in (8.1) is

$$\sum_{i=0}^{s} \alpha_i m_{n+i} = \Delta t \sum_{i=0}^{s} \beta_i \tau(m_{n+i}, t_{n+i}), \quad (8.4)$$

where $m_n = m(t_n)$, and $t_n$ represents the time at step $n$, which, assuming a fixed time step $\Delta t$, is $t_n = t_0 + n\Delta t$, $t_0$ being the initial time. The values of $\alpha_i$, $\beta_i$, and $s$ define the particular linear multistep method. In its generalized form (8.4), the LMM formula provides a relation between the magnetization $m_{n+s}$ at time $t_{n+s}$ and the magnetization at previous $s$ steps ($m_{n+i}$ for $0 \leq i \leq s - 1$). The relation is in the form of a linear combination of $m_{n+i}$ and $\tau_{n+i}$, from which $m_{n+s}$ may, in one manner or another, be obtained. Once $m_{n+s}$ is found, a new step may be taken and the scheme repeated iteratively to yield the evolution of the magnetization vector $m$.

We next discuss different families of LMMs, specified by different values of $\alpha_i$ and $\beta_i$, and describe the determination of $m_{n+s}$ from the respective formulas.
Adam-Bashforth Methods

The Adams-Bashforth methods are derived from Eq. (8.4) by imposing \( \alpha_s = 1 \), \( \alpha_{s-1} = -1 \), \( \alpha_{s-i} = 0 \) for \( 2 \leq i \leq s \), and \( \beta_s = 0 \). The latter imposition renders the methods explicit as it expels \( m_{n+s} \) from the argument of vector function \( \tau \) on the right-hand side of Eq. (8.4). The general formula for Adams-Bashforth methods, therefore, is

\[
m_{n+s} = m_{n+s-1} + \Delta t \sum_{i=0}^{s-1} \beta_i \tau(m_{n+i}, t_{n+i}).
\] (8.5)

The value of the constant \( s \) specifies the number of previous steps included in the evolution of \( m_{n+s} \), and also determines the order of the method. The values of constants \( \beta_i \) are order dependent, and can be derived using polynomial interpolation [Hindmarsh and Serban, 2007] as

\[
\beta_{s-j-1} = \frac{(-1)^j}{j!(s-j-1)!} \int_0^1 \frac{1}{j!} \prod_{i=0, i\neq j}^{s-1} (u + i) \, du, \quad j = 0, 1, \ldots, s-1.
\] (8.6)

For \( s = 1 \), Eq. (8.6) reduces to the one-step Euler method

\[
m_{n+1} = m_n + \Delta t \, \tau(m_n, t_n).
\] (8.7)

In micromagnetics, for nonstiff problems, the fourth order \( (s = 4) \) Adams-Bashforth formula is commonly used,

\[
m_{n+4} = m_{n+3} + \Delta t \left[ \frac{55}{24} \tau(m_{n+3}, t_{n+3}) - \frac{59}{24} \tau(m_{n+2}, t_{n+2}) 
+ \frac{37}{24} \tau(m_{n+1}, t_{n+1}) - \frac{3}{8} \tau(m_n, t_n) \right],
\] (8.8)

as it combines accuracy with low implementational complexity.

Adam-Moulton Methods

Following the same procedure used in deriving the Adams-Bashforth formulas from Eq. (8.4), but doing away with the imposition \( \beta_s = 0 \), one arrives at the Adams-Moulton formulas

\[
m_{n+s} = m_{n+s-1} + \Delta t \beta_s \tau(m_{n+s}, t_{n+s}) + \Delta t \sum_{i=0}^{s-1} \beta_i \tau(m_{n+i}, t_{n+i}).
\] (8.9)
The second (new) term on the right-hand side of the above equality makes the Adams-Moulton methods implicit. The vector \( \mathbf{m}_{n+s} \) can be found from the implicit formula using Newton’s method (see section 8.2.3 on solutions to implicit equations). To accelerate convergence to the solution, a good initial guess can be provided to Newton’s method by the (explicit) Adams-Bashforth methods. This two-method scheme is known as the predictor-corrector method. For comparison to the Adams-Bashforth formulas for \( s = 1 \) (8.7) and \( s = 4 \) (8.8), the Adams-Moulton formulas for the same values of \( s \) are

\[
\mathbf{m}_n = \mathbf{m}_{n-1} + \Delta t \tau(t_n),
\]

\[
\mathbf{m}_{n+1} = \mathbf{m}_{n+3} + \Delta t \left[ \frac{251}{720} \tau(t_n, t_{n+4}) + \frac{646}{720} \tau(t_n + 3, t_{n+3}) - \frac{264}{720} \tau(t_n + 2, t_{n+2}) + \frac{106}{720} \tau(t_{n+1}, t_{n+1}) - \frac{19}{720} \tau(t_n, t_n) \right].
\]

Equation (8.10) can be recognized to be the backward Euler method.

For an arbitrary step parameter \( s \), the coefficients \( \beta_i \) are given as

\[
\beta_{s-j} = \frac{(-1)^j}{j! (s-j)!} \int_0^1 \prod_{i=0}^s (u + i - 1) \, du, \quad j = 0, 1, \ldots, s.
\]

Backwards Differentiation Formulas

Starting from Eq. (8.4) and imposing the condition \( \beta_{s-i} = 0 \) for \( 1 \leq i \leq s \), one arrives at the general expression for the backwards differentiation formulas (BDFs)

\[
\sum_{i=0}^s \alpha_i \mathbf{m}_{n+i} = \Delta t \beta_0 \tau(t_n, t_{n+s}).
\]

For comparison with Adams-Bashforth formulas (8.7) and (8.8), and Adams-Moulton formulas (8.10) and (8.11), the BDFs for \( s = 1 \) and \( s = 4 \) are

\[
\mathbf{m}_{n+1} - \mathbf{m}_n = \Delta t \tau(t_{n+1}, t_{n+1}),
\]

\[
\frac{25}{12} \mathbf{m}_{n+1} - 4 \mathbf{m}_n + 3 \mathbf{m}_{n-1} - \frac{4}{3} \mathbf{m}_{n-2} + \frac{1}{4} \mathbf{m}_{n-3} = \Delta t \tau(t_{n+1}, t_{n+1}).
\]

While Adams methods are more suited to nonstiff problems, where they provide more accurate solutions than BDFs for the same order and computational time, the opposite is true for the case of stiff problems. Sophisticated implementations of the
BDF method include variable time-stepping and variable order, which can tremendously increase numerical integration speed. A synopsis can be found in [Cohen and Hindmarsh, 1996, Cohen and Hindmarsh, 1994, Hindmarsh and Serban, 2007]. Lastly, we note, since the BDF method is implicit, the method’s overall efficiency is intimately dependent on the efficiency of the technique used to solve the implicit system, thus motivating the discussion of the Jacobian-free Newton-Krylov method in section 8.2.3.

8.2.2 Implicit Midpoint Formula

The LLMs described in the previous sections (BDFs in particular) are superb time-stepping techniques for the study of magnetization processes such as magnetization relaxation to equilibrium states, domain wall nucleation, magnetic recording on film, reversal modes in nanostructures, and energy barrier calculations using the nudge elastic band method (section 6.2). However, in other types of studies, including studies of resonance properties, steady-state precession, vortex oscillations, spin-wave dynamics, and other processes where key features of magnetization response can show high sensitivity to the slightest variations of system energy, greater care must be taken when using LMMs to ensure the preservation of the magnetization magnitude during simulation and prevent artificial energy dissipation/pumping due to numerical truncation error implicit to the time-stepping schemes. This involves limiting the maximum allowed time step, decreasing tolerances, and adjusting many other optimization parameters implicit to the method in a judicious manner, which can be nontrivial and can lead to considerably reduced integration speed. For this reason, geometric integration techniques have been sought which inherently preserve the key properties of the LLG equation ([d’Aquino et al., 2005] and references therein).

The implicit midpoint formula was identified to simultaneously preserve the magnetization magnitude, Lyapunov structure, and system energy (in case of zero damping), regardless of the step size, thus facilitating the geometric integration of the LLG equation [d’Aquino et al., 2005]. The implicit midpoint formula, applied to the (implicit) Gilbert form of the LLG equation (2.2), yields

$$\frac{\mathbf{m}_{n+1} - \mathbf{m}_n}{\Delta t} = -\gamma \frac{\mathbf{m}_{n+1} + \mathbf{m}_n}{2} \times \left[ \mathbf{H}_{\text{eff}} \left( \frac{\mathbf{m}_{n+1} + \mathbf{m}_n}{2}, t_n + \frac{\Delta t}{2} \right) - \alpha \frac{\mathbf{m}_{n+1} - \mathbf{m}_n}{\Delta t} \right],$$

(8.16)

where \( \mathbf{m} \) is a composite vector consisting of the unit magnetization vectors associated with all \( N \) mesh nodes of the discretized system, i.e., \( \mathbf{m} = [\hat{\mathbf{m}}_1 \hat{\mathbf{m}}_2 \hat{\mathbf{m}}_3 \ldots \hat{\mathbf{m}}_N] \), and \( \mathbf{H}_{\text{eff}} \)
is a composite vector of equivalent structure. Examining the equation above [d’Aquino et al., 2005], it can easily be shown that $|m_{n+1}|^2 - |m_n|^2 = 0$, implying the conservation of magnetization magnitude. For constant applied field, it can be proved that the energy necessarily decreases with time, $\frac{E(m_{n+1}) - E(m_n)}{\Delta t} = \alpha \left| \frac{m_{n+1} - m_n}{\Delta t} \right|^2$, indicating that the implicit midpoint formula preserves the Lyapunov structure. Lastly, in the absence of dissipation ($\alpha = 0$), the implicit midpoint formula can be shown to preserve constant system energy to within an error of $O(\Delta t^3)$.

The implicit nature of the discussed method necessitates the solution of a nonlinear system of equations, as is also required by the Adams-Moulton methods and the BDFs, more on which is to be found in the following section.

8.2.3 Jacobian-Free Newton-Krylov Methods

Implicit methods covered in the preceding sections, (8.9), (8.13), (8.16), can all be reformulated as

$$F(m_{n+s}) = 0, \quad (8.17)$$

with all known terms, including $m_{n+i}$ for $0 \leq i \leq s - 1$, and time(s), treated as constants and hence omitted from the argument of the vector function $F$. Since the function $F$ is generally nonlinear in $m_{n+s}$ (since it involves $\tau(m_{n+s}, t_{n+s})$; see (8.1)), Newton’s method may be used to linearize the system and iteratively search for the solution $m_{n+s}$ satisfying (8.17).

Dropping the subscript $n + s$ (which is fixed during the Newton iterations), introducing a superscript $k$ to denote the Newton iteration number, and defining $F'(m) = \frac{\delta F(m)}{\delta m}$, we derive Newton’s method from the first order Taylor expansion of $F$ about $m^{k+1}$,

$$F(m^{k+1}) = F(m^k) + F'(m^k)(m^{k+1} - m^k). \quad (8.18)$$

Setting $F(m^{k+1}) = 0$ yields

$$J(m^k) \delta m^k = -F(m^k), \quad (8.19)$$

where $J(m) = F'(m)$ is the Jacobian, and

$$\delta m^k = m^{k+1} - m^k \quad (8.20)$$

represents the Newton correction, sought during each iteration to achieve convergence in satisfaction of (8.17).
Recalling that $m^k$ represents the composite vector of the three spatial components of all the $(N)$ mesh nodes of the discretized system (8.2), and that $F$ represents the composite vector of equivalent structure, $J$ in (8.19) can be recognized to be a $3N \times 3N$ Jacobian matrix. The Krylov subspace at iteration $j$ for the system given in (8.19) is

$$K_j = \left\{ r_0, \, Jr_0, \, J^2r_0, \ldots, J^{j-1}r_0 \right\},$$

(8.21)

where the initial linear residual is obtained as

$$r_0 = -F(m) - J\delta m_0,$$

(8.22)

and $\delta m_0$ is the initial guess for the correction $\delta m$. The superscript $k$ has been omitted because its value is fixed at each Krylov iteration. Since subspace $K_j$ only includes maps of $r_0$ produced by the action of $J^i$ for $0 \leq i \leq j - 1$, the values of the $6N^2$ elements of the Jacobian matrix need not be explicitly known. The vectors $J^i r_0$ for $0 \leq i \leq j - 1$ are what is explicitly needed. For this reason, the use of Krylov subspace methods in conjunction with Newton’s method is referred to as the Jacobian-free Newton-Krylov (JFNK) method. The great advantage of the JFNK method is that the need to construct the full system Jacobian is eliminated, as long as vectors $J^i r_0$ for $0 \leq i \leq j - 1$ are provided.

The typical choice for the initial guess for the Newton correction $\delta m_0$ in (8.22) is zero. At each new iteration $j$, $\delta m_j$ is obtained as a linear combination of basis vectors from $K_j$,

$$\delta m_j = \delta m_0 + \sum_{i=0}^{j-1} \beta_i J^i r_0,$$

(8.23)

with coefficients $\beta_i$ chosen to minimize the residual $r_j = |F(m) + J\delta m_j|$. The generalized minimal residual method (GMRES) can be used to optimize the residual minimization process based on a variation of the principles outlined.

The matrix-vector products necessary to construct the subspace of basis vectors which are used to form the Newton correction can be expressed through the limit [Knoll and Keyes, 2004]

$$Jv = \lim_{\varepsilon \to 0} \frac{F(m + \varepsilon v) - F(m)}{\varepsilon}.$$

(8.24)

Recently, it has been shown that for the case of micromagnetics, where $F$ reflects the structure of the LLG equation or one of its variants, an analytical expression can be derived from (8.24), which provides a means to construct Krylov subspaces at a greater speed and accuracy than possible by using finite differences, thus improving JFNK
performance and LLG integration efficiency, when using implicit methods such as BDF. For detailed derivations and proofs pertaining to the improved analytical method the reader is referred to [Chang et al., 2012b, Escobar et al., 2012a].

8.3 Vector Computing on Graphics Processing Units

While large-scale computer simulations may be capable of providing precious insight into the complicated dynamics of many physical systems, the computational time required to obtain the solution is far too often all too dear. Since most physics simulators primarily toil over matrix-matrix or matrix-vector products, efficient ways to accelerate arithmetic operations involving large data structures at the hardware level have always been of importance. Indeed, conventional central processing units (CPUs) are a general-purpose architecture, not optimized for high-performance basic arithmetic. For this task, specialized vector computing clusters were in production early on, but the development of the technology was not on par with the booming of the CPU and personal computer industry, and ultimately CPUs became the sole instrumentality of scientific computing.

The increasing popularity of video games and the fortuitous expansion of the gaming industry in the years to follow paved the way to new highs in textured 3D video rendering, and concomitantly, scientific computing. The vast consumer market and sustainability of the GPU technology propelled the development of the massively parallel GPU architecture, facilitating blistering array arithmetic and image processing. Molecular dynamics, quantum chemistry, Battlefield 3, and Deus Ex: Human Revolution, could now all be run on highly optimized hardware at speeds simply unapproachable by CPUs alone.

The great advantages of GPU vector computing are owed to the significantly higher number of specialized cores, simplified processing, limited communication with remote memories, and far increased bandwidth in comparison with CPUs. The improvement in performance is especially welcome considering GPUs come at a bargain cost of $\sim 500$ a pop for the average model, while offering orders of magnitude speedups for certain operations.

However, running scientific simulations on GPUs is not a simple matter of plug-and-play. Codes must be specifically written and optimized to run on GPUs. This has been done for our micromagnetic simulator FastMag [Li et al., 2010, Chang et al.,
The calculation of the micromagnetic fields, currents, and torques, presented in chapters 3–7, can all be cast in the form of matrix vector products [Chang et al., 2011] whose evaluation can be performed on GPUs [Li et al., 2011]. Numerical integration algorithms can also be ported to GPUs. Of course, a mild dependence on CPUs still remains, associated primarily with the preprocessing stages and other incidental parts of the code.

While the CPU portions of the code are written in C/C++ or Fortran, the GPU part is developed in the CUDA or OpenCL environment. Proficient understanding of the GPU architecture is required for developing codes that take maximum advantage of the massively parallel computing platform. Careful considerations of data structures, memory handling, and data transfer are central to efficient GPU-based programming. For more information on GPU accelerated micromagnetics, including a GPU versus CPU performance comparison, we refer the interested reader to the work of S. Li et al. [Li et al., 2010, Li et al., 2012, Li, 2012].

In closing, we stress our belief that GPU technology will continue to provide opportunities for scientific computing in the comfortable future. Leading developers have already launched several scientific-specific GPU models which harbor more memory than their gaming counterparts, and sport less gaming-specific components. More and more high-level packages and libraries are becoming available as well, including matrix equation solvers useful for numerical integration, and possibly highly sophisticated numerical integration modules such as CVODE [Cohen and Hindmarsh, 1996].

### 8.4 Parallelization

A discussion of acceleration schemes for micromagnetic solvers would not be complete without addressing parallelization. In the evaluation of effective magnetic fields, currents, and torques at each time step during the numerical solution of the LLG equation (or one of its modifications), much of the computation can be divided into segments which can be executed independently. Concurrent execution of discrete parts of the problem over multiple processors typically leads to orders of magnitude speedups in comparison to serial computing, provided the problem is partible and the problem size large enough to offset inter-processor communication costs. Since the bulk of the computational effort for the micromagnetic solvers described in the preceding chapters is concentrated on GPUs (section 8.3), it is natural to consider multi-GPU parallelization as a means of furthering
gains in computational speed for problems involving millions or billions of unknowns. Even if maximally boosting speed is not one’s primary aim, the combined power of multiple GPUs is still important in providing the needed memory for large simulations, where cumbrous arrays pertaining to the discretized system cannot be received by the memory onboard a single unit.

Many considerations pertaining to multi-GPU parallelization resemble those of conventional CPU-parallelization. These include memory loading, task scheduling, and data exchange across multiple units. Their optimization is essential for maximizing parallelization efficiency. Portability is another key consideration. Code efficiency should not be overly dependent on the specifics of any given GPU model, as device architectures are bound to change generationally. More on multi-GPU parallelization in the context of micromagnetic solvers can be found in [Li et al., 2011, Fu et al., 2013].
Part III

Micromagnetic System Analysis
9 Perpendicular Magnetic Recording

The present chapter begins with a brief history of magnetic recording. Key technological advances responsible for driving up storage capacities are outlined. Outstanding challenges for further improvements in recording density are examined. Design considerations for advanced write heads are discussed in reference to our recent micromagnetic study [Escobar et al., 2012b]. Prospective alterations to the media platform and recording scheme, envisioned to significantly extend areal densities, are described. Simulations of magnetic recording on granular strips are presented [Lubarda et al., 2011a, Lubarda et al., 2012a], which were based on the models developed in chapter 7. Recorded patterns obtained from simulations are analyzed for signal quality. The procedure adopted for signal analysis is described.

9.1 Introduction to Magnetic Recording

9.1.1 Early History

The first scientific article on magnetic recording was published in the United Kingdom in 1888. Its author was Oberlin Smith, a Cincinnati born engineer, who, in his 1888 letter, outlined the possibility of data storage based on a magnetic imprinting technique whereby steel dust particles suspended within a cotton thread would be magnetized by a single pole transducer [Smith, 1888]. However, a formal demonstration of the idea never followed.

Magnetic recording in its earliest form was officially demonstrated in 1898 by the Danish engineer Valdemar Poulsen, who immediately patented his invention. It was the magnetic wire recorder, envisioned to serve as a general voice recording apparatus, and
provide a pathway to technologies such as an automated telephone answering machine. The original invention employed a magnetic wire as the recording medium. Later, magnetic tape was used, followed by oxide media, and more recently magnetic thin film heterostructures and patterned nanoscale pillars, with numerous patents marking each advancement to improved recording capability.

The first moving head disk drive in a computer was implemented by the New York-based company IBM (International Business Machines) in 1956. The computer system, 305 RAMAC, had a data storage capacity of 4.4 MB, corresponding to an effective areal density of 2 kb/in² at the time [McFadyen et al., 2006]. This stands in stark contrast to the 500 Gb/in² of today’s disk drives. The following sections outline the technological advances that have led to increasing areal density, and describe the obstacles that must be overcome for further progress to be made.

9.1.2 Moore’s Law

Moore’s law for magnetic recording technology states that approximately every two years the information storage capacity of magnetic memory devices is doubled. Indeed, a roughly steady exponential progression rate is evidenced from the areal densities of retail products over the past few decades. However, this seemingly consistent pace of increasing storage capacity is not, by and large, due to continuous gradual improvements in the same technology, but is rather propelled by abrupt discoveries and innovations [Moser et al., 2002], whose impact on areal densities are not always instantaneously experienced due to the time required for product development and maturation.

Despite surprising discoveries and cutting edge innovations that made the advance to greater areal densities possible, much about the dimensions and properties of the components of the new generation systems could be foreseen from simple scaling analysis. Understanding how areal density, fields, and current densities scale with length, it is possible to show [McFadyen et al., 2006] how information pertaining to media thickness, fly height, and read head properties, at some future areal density, could be estimated with admirable accuracy from the corresponding values of the primordial 305 RAMAC disk drive sporting a 2 kB/in² capacity.
9.1.3 Key Technological Advances

Thin Films

The earliest notable advancement in magnetic recording technology was the transition from particulate to thin film materials which occurred in the 1980s. The transition was occasioned by the need for a more scalable media platform, since particle size in particulate media could not be further reduced without significant deterioration to media quality. Sputtered thin films proved to be the superior media platform, due to their granular microstructure and tunable grain properties and distributions.

The granular microstructure of thin-film media is shown schematically in Fig. 9.1. In granular media, each bit consists of a cluster of grains whose magnetic moments have a positive component in one of the two defining directions. In Fig. 9.1 the two defining directions are left and right, corresponding to binary values of 1 and 0, respectively. Since the magnetization of the grains is in-plane with respect to the film, this media is called longitudinal media. Due to the small bits supported by the granular structure of magnetic thin films, miniaturized recording heads were developed at the microscopic scale to take full advantage of the new media. Multilayer thin films with out-of-plane magnetization eventually replaced longitudinal media, a discussion of which will follow.

Readback Technology

Additional increases in areal densities came with the modernization of read head technology. Early read heads that flew over the media translated the magnetization direction of the bits to a voltage signal via magnetic inductance. Initially, a single
inductive head was used to do both the reading and writing. Due to the poor scalability of such a design, new read heads were developed in the early 1990s whose operation was based on the anisotropic magnetoresistance effect (AMR). In this design, a soft magnetic element in the read head aligns with the magnetization of the media owing to magnetostatic coupling. The magnetization state of the soft element is subsequently determined by a voltage readout differing by 1–2%, depending on the orientation of the magnetization of the element with respect to the current direction.

Though AMR heads were a significant improvement over inductive sensors, it was only with the introduction of read heads based on the giant magnetoresistance effect (GMR) in the late 1990s that the limitation posed by readback on the achievable areal densities was significantly offset. The magnetoresistance ratio of GMR was an order of magnitude greater than that of AMR. Further advancements were made with the introduction of read heads consisting of magnetic tunnel junctions (MTJs) and a transition from current in-plane (CIP) geometry to current perpendicular-to-plane (CPP) geometry. Technological implications of GMR and TMR effects are discussed in more detail in section 12.1.

Transition from Longitudinal to Perpendicular Magnetic Recording

Longitudinal magnetic recording (LMR), together with materials advances and improved read head technology, took areal densities of recording media to 100 Gb/in² by around 2006. Scalability of LMR beyond this mark faced a number of challenges. The anisotropy energy density $K$ of quality materials with an in-plane easy axis was not sufficiently high to support further scaling down of grains. Since the thermal stability of the grain is given by the product of anisotropy energy density and grain volume $KV$, reducing the grain size without increasing $K$ would make the media susceptible to thermal fluctuations that can reverse the grain magnetization. Spontaneous switching of unstable magnetic particles in the presence of thermal fluctuations is known as the superparamagnetic effect. Superparamagnetism results in rapid deterioration of the magnetically stored data. To ensure at least 10 years of data retention near room temperature, the thermal stability product needs to be $KV \gtrsim 60k_B T$, where $k_B$ is the Boltzmann constant and $T = 300$ K.

Another problem with LMR was that the dipolar (magnetostatic) interactions between the bits were very large due to the in-plane magnetization of the grains (Fig.
In particular, the head-to-head and tail-to-tail configurations destabilize the bits and can lead to subsequent reorientation to the more stable head-to-tail configuration, thereby compromising information integrity.

Longitudinal recording on high density media was also limited by the field gradients of the double-pole write head. For high density recording, large field gradients are required for writing sharp transitions, which the longitudinal recording head models could not provide.

The summarized problems facing additional increases in areal density of longitudinal recording media motivated the transition to perpendicular magnetic recording (PMR) systems in the second half of the 2000s. The media used in PMR is typically a granular multilayer heterostructure (section 11.3) having an overall perpendicular magnetic anisotropy (PMA) so that the easy axis is vertical to the film and the magnetization points out of plane. The PMA energy density $K$ of multilayer heterostructures such as Co/Pt, Co/Pd, or Fe/Pt can be extremely high, which allows grains to be additionally scaled down without jeopardizing thermal stability. Other PMA materials of high uniaxial energy density include Co$_3$Pt, ordered L1$_0$ FePt, FePd, and CoPt, and rare earth transition metals Nd$_2$Fe$_{14}$B and SmCo$_5$.

A further advantage of PMR is that the dipolar interactions between neighboring bits are reduced because aligned head-to-head and tail-to-tail configurations are not encountered. Additionally, in PMR, a single-pole recording head can be used together with the soft underlayer (SUL), which resides beneath the media and acts as a magnetic mirror, to achieve large field gradients and strong write fields required to write sharp transitions on the hard perpendicular media [Khizroev and Litvinov, 2004]. Magnetic shields can be used to improve recording resolution by further increasing the write field gradients to achieve sharper bit transitions [Mallary et al., 2002, Takano, 2005, Okada et al., 2005, Ise et al., 2006, Kanai et al., 2010, Tagawa et al., 2012]. This was confirmed by our recent study of the effects of wraparound shields (WAS) on system performance [Escobar et al., 2012b].

The improvement in write field gradients on account of the WAS can be observed by contrasting Fig. 9.2a and 9.2b which show the profile of the $z$-component of the write field for a model with and without a WAS. The write field profiles were obtained by evaluating the stray field generated by the single-pole recording head over a $300 \times 300$ nm area, 12 nm below the air bearing surface (ABS). The smooth transition from red to
yellow in Fig. 9.2a, relative to the sharp change in color observed in Fig. 9.2b, indicates that in the presence of the WAS the write field gradients are substantially greater.

While shields can significantly improve field gradients in PMR, the magnitude of the field typically suffers. Careful optimizations must be performed to maximize gradients without jeopardizing writability. Other possible adverse effects of shields include adjacent (ATE) or far track erasure (FTE). Figure 9.3a shows a snapshot of the write field profile evaluated over a 0.8 μm × 1.0 μm area, situated 12 nm below the ABS, extending beneath both the pole tip and the WAS. Large fluctuations of the stray field are seen to occur beneath the WAS. The amplitude of the fluctuations can reach a few kOe in regions

Figure 9.2: Recording field profile 12 nm under the air bearing surface generated by a PMR write head (a) with no wraparound shield, and (b) with wraparound shield.
both close and far to the pole tip. Such large fields can lower the energy barrier for thermally activated reversal and thus lead to ATE or FTE. These deleterious fields can be attributed to domain wall processes in the WAS, as reported elsewhere [Song et al., 2009], and as evidenced by Fig. 9.3b, showing magnetization of the shield at the surface. Design solutions to eliminate sources of ATE and FTE, while maintaining strong field gradients, are a matter of ongoing investigation for extending areal densities of PMR.

**Acknowledgements:** Section 9.1.3 in Chapter 9, in part, is based on the journal article: M. E. Escobar, M. V. Lubarda, S. Li, R. Chang, B. Livshitz, V. Lomakin, “Advanced micromagnetic analysis of write head dynamics using FastMag,” *IEEE Transactions on Magnetics* 45 (5), 1731–1737 (2012). The dissertation author was the contributing author to this article.

### 9.1.4 Future Prospects for Magnetic Recording

Further downscaling of the perpendicular magnetic recording system without some fundamental change in the recording process or media design will be difficult due to several reasons, which together are familiarly known as the magnetic recording trilemma. The trilemma pertains to three focal aspects of magnetic recording: areal density, thermal stability, and writability. The three aspects are frustrated in the sense that improvement in one aspect results in degradation elsewhere. Reducing grain size to increase the
areal density diminishes the thermal stability. Increasing anisotropy to improve stability increases the coercivity. High coercivity would not be problematic if fields of arbitrary intensity could be supplied by the recording heads. Unfortunately, the maximal field generated by a writer is limited by the saturation magnetization $M_s$ of the pole tip. Today’s recording heads, used in $\sim 500$ Gb/in$^2$ recording, have a tip of $M_s \approx 2000$ emu/cm$^3$, which is close to the highest $M_s$ of a known material. The resulting recording field intensity is around 15 kOe. A media coercivity exceeding this value constitutes a writability problem. Scaling down to higher areal densities will involve the miniaturization of the recording head which is expected to exacerbate the writability problem due to (i) the weaker fields generated by smaller heads and (ii) increased media anisotropy needed at higher density. Further enhancements in storage capacity must, therefore, involve a departure from the conventionally followed scaling routine. Several ideas have been proposed to remedy the situation described by the trilemma. We summarize five of these ideas, one of which has already been implemented, while the remaining are being extensively researched both in industry and academia.

The first of these ideas comes from the investigation of spring media. Spring media represents two or more magnetic layers exchange coupled either directly or across a spacer layer. It was demonstrated that if a magnetically hard layer is coupled to a softer layer, the reversal field needed to switch the magnetization of the composite is much lower than that required to switch the magnetization of the hard layer alone [Fullerton et al., 1998, Fullerton et al., 1999]. This is due to the spring-like configuration of the exchange coupled composite which allows the soft layer to respond more readily to the external field and supply an additional torque to the hard layer, assisting its reversal [Suess et al., 2005, Victora and Shen, 2005a]. The greatest reduction in switching field is achieved for a choice of material and structural properties that promotes domain wall nucleation in the soft layer followed by domain wall injection into the hard layer [Suess, 2007]. It was shown that, while the switching field of the composite structure can be reduced two to six times with respect to the hard layer alone, the thermal stability is not necessarily affected. This substantial decoupling between writability and stability can be traced back to the qualitative difference between the field-driven reversal mode and the thermal reversal mode [Suess et al., 2005]. The magnetic recording industry has already employed this design, which is commonly known as the exchange coupled composite media or ECC media.
An extension of this design has also been proposed, called graded media, which consists of multiple layers of different anisotropies stacked to result in an anisotropy gradient [Goncharov et al., 2007]. For a specific gradient profile it was shown that, in principle, an infinitesimally small field is sufficient to reverse the stack. Other extensions of the spring media concept have also been proposed, some of which are presented in section 11.4 and 11.5.

Though ECC media helps improve writability, it does not offer indefinite gains, and other approaches have been proposed to take recording to yet greater areal densities. The premiere among these is heat assisted magnetic recording (HAMR), also known as thermally (or energy) assisted recording [McDaniel, 2005]. The main idea behind HAMR is to take advantage of the temperature dependence of the material properties of magnetic media. Heat can be delivered locally to the medium by use of a miniaturized laser or near field optical transducer, which increases the temperature of the portion of the media that needs to be written. Since the magnetic anisotropy falls off with increasing temperature, the targeted region is magnetically softer and easier to write.

The optimal temperature for heat-assisted switching is estimated to be around $T_C$. The reversal process involving heat-assist significantly differs from reversal at constant ambient temperatures. As the temperature rises toward $T_C$, the atomic spins become quickly disoriented, the net macroscopic magnetic moment density with no field applied approaches zero, and the susceptibility to an applied magnetic field greatly increases. Using the magnetic head field to bias the spins in a given direction, and discontinuing heat delivery thereafter, allows the magnetization to stabilize along the prescribed direction as the material cools and the magnetic anisotropy recovers. The heat-assisted scheme could allow writing on high anisotropy media at record areal densities, resolving the magnetic recording trilemma. Extensive effort has been dedicated to the research of heat assisted recording followed by a number of recent recording demonstrations [Rottmayer et al., 2006, Seigler et al., 2008, Kryder et al., 2008, Challener et al., 2009, Stipe et al., 2010, Stipe et al., 2011]. Still more work is needed before the technology can replace conventional magnetic recording. More on HAMR can be found in chapter 10.

An alternative to HAMR is microwave assisted magnetic recording (MAMR). In MAMR, in addition to the DC magnetic field produced by the recording head, a supplementary microwave field in the GHz frequency range is used to assist reversal [Zhu et al., 2008]. The microwave field frequency must match the ferromagnetic resonance of
the media so that energy is efficiently supplied to the system to induce reversal. The magnetization dynamics associated with the reversal is similar to Rabi oscillations of spins in molecules during magnetic resonance imaging (MRI), albeit the resonance frequency of the two is much different. STNOs can generate local microwave fields in the GHz range with reasonably narrow bandwidths, and thus are a promising microwave source for MAMR. One key challenge that remains is the low power output of STNOs. Section 12.1.4 offers a more elaborate discussion on this topic.

All schemes depicted so far were a modification or extension to the conventional magnetic recording process, but did not involve absolute structural changes to the recording medium. One approach aims to improve the areal densities specifically by altering the medium architecture. The alteration consists of patterning a continuous granular medium into an array of closely spaced nanoislands [Shiroishi et al., 2009]. The key difference between continuous granular and patterned media is that the former has an irregular microstructure necessitating the incorporation of many grains in a bit for a sufficient signal-to-noise ratio (SNR), while the latter has a periodic structure allowing each nanoisland to store a single bit of information, thus achieving higher storage capacity, and improving SNR owing to strict periodicity. The areal density that can be achieved by patterning continuous recording media can be increased even further by taking advantage of domain wall assisted reversal or thermal assist, as discussed earlier in this section. More about patterned media can be found in chapter 11.

9.2 Recording Simulations and Bit Pattern Analysis

While many strategies have been proposed to extend areal density limits of conventional PMR, including heat-assisted writing and bit patterning, understanding how the signal quality depends on structural and material parameters of the media, the write head profile, and the read head design as grains are further downscaled, remains critical not only for achieving gains in PMR areal densities in the short term, but also for providing the insight necessary to most efficaciously transition to a new recording regime, such as HAMR or MAMR. In the following sections, we present micromagnetic simulations of recording on continuous granular media, and describe our approach for investigating signal quality.
Figure 9.4: Three spatial components of the write field which are used to record transitions.

9.2.1 Granular Media Model

Single-layer granular strips having a cross-track width of 200 nm and a down-track length ranging from 1μm to 12μm are considered. The granular microstructure of the strips was obtained via Voronoi tessellation, segregation, and extrusion processes. Details of the modeling procedure are described in section 7.2. The average grain diameter in each model was chosen to be ⟨d⟩ = 7.1 nm. All Voronoi cells have been extruded from corresponding Voronoi diagrams to result in a uniform strip thickness of t = 12 nm. The shortest 1μm long recording strip contains 4304 grains. The largest 12μm strip contains 48292 grains. In the models, each grain is treated as a marospin particle. This approximation is appropriate, since the grain dimensions fall below the exchange length. The exchange stiffness, saturation magnetization, perpendicular uniaxial anisotropy energy density, and damping used for the models are $A_{ex} = 1.0 \, \mu\text{erg/cm}$, $M_s = 660 \, \text{emu/cm}^3$, $K_u = 3.63 \, \text{Merg/cm}^3$ and $\alpha = 0.1$. We have chosen to introduce variations in the easy axis direction of the grains in each model. The variation for all recording strips is characterized by a Gaussian distribution with a mean and standard deviation of the easy axis given in polar coordinates (θ, φ) as $\mu_\theta = 0^\circ$, $\sigma_\theta = 2^\circ$, and a uniform (flat) distribution in φ (the azimuthal angle). The intergranular exchange coupling is given by the interface energy density $J = 0.07 \, \text{erg/cm}^2$, which translates to an effective strip stiffness of $A_{ex}^{eff} = 0.05 \, \mu\text{erg/cm}$, corresponding to approximately 5% of the bulk (intragranular) exchange constant.
Figure 9.5: Bit pattern recorded on a 9 µm granular strip. Zoom-in shows the action of the write field as the recording head writes in the last few transitions.

9.2.2 Head Field Model

A precomputed head field profile was provided to the micromagnetic solver in the form of a tabulated input file obtained from a calculation of the stray field generated below the air bearing surface of a recording head. (Similar calculations are presented in [Escobar et al., 2012b]). The three spatial components of the head field are shown in Fig. 9.4. The peak amplitude is 11 kOe in the vertical direction. In each of the simulations presented next, the relative velocity of the head with respect to the media is \( v = 20 \) m/s. The switching of the head was chosen to be periodic, to facilitate signal analysis using the procedure outlined in section 9.2.4. The switching period was chosen to be 2 ns with a time modulation of the form \( e^{-t/\tau} \), and a rise time of \( \tau = 0.2 \) ns. Such specifications translate to the writing of one bit every 1 ns at a linear density of 1270 kfc.

9.2.3 Recording Simulations

Strip models of different lengths described in section 9.2.1, together with the head field profile described in section 9.2.2, were used to micromagnetically simulate the recording of periodic patterns, which were subsequently analyzed for signal quality. The anisotropy, intergranular exchange, magnetostatic, and applied fields acting on each grain of the recording strips were accounted for according to formulas and procedures described in section 7.5. The numerical integration of the LLG equation was performed using the
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Figure 9.6: (a) Readback signal (black curve) obtained from the recording shown in Fig. 9.5; perfectly periodic fit (red curve) to the signal. (b) Signal (black curve) and noise (red curve) power versus linear density for the same recording.

Adams-Bashforth forth-order algorithm, outlined in section 8.2.1. Figure 9.5 shows the bit pattern on a granular strip of 9 µm in length, as the recording head writes in the last few transitions.

9.2.4 Signals Analysis

While Voronoi modeling, presented in section 7.3, enables accurate representation of the magnetic recording medium, and while the micromagnetic solver described in section 7.5 allows for efficient simulations of the magnetic recording process, suitable methods must be developed for the analysis of the signal quality of recorded patterns. With the ability to properly analyze signal quality, SNR versus areal density characteristics can be rigorously studied and information deduced on how to best optimize media and the recording process for maximum storage capacity [Bertram and Williams, 2000]. Material and structural parameters of the media, including grain size, $K_u$, $M_s$, $J_{ex}$,
Figure 9.7: Plot of transition misplacement for the first few hundred transitions of the recording shown in Fig. 9.5: histogram graphically representing the transition misplacement distribution, the standard deviation of which quantifies the jitter.

and the distributions therein, together with the head field profile, switching rate, write mode (e.g., shingled recording, assisted recording), and read head design, represent key factors affecting the SNR versus bit density characteristic. Advanced modeling capability, powerful micromagnetic solvers, and robust signal analysis techniques, therefore, form the ultimate tool for computationally probing the areal density limits of magnetic recording technology.

In this section we describe the procedure used to analyze the signals of recording patterns, as the one shown in Fig. 9.5. The procedure we follow is similar to that performed in spin stand studies. Figure 9.6a shows the raw waveform (black curve) from the readback process with noise, and a perfectly periodic fit to the signal (red curve). The raw signal was obtained by projecting the magnetization to a uniform grid and convoluting it with the readback sensitivity potential calculated for a particular head model [Yuan and Bertram, 1994].

Figure 9.6b shows the signal and noise power versus linear density for the 9 µm recording. The signal power is obtained by fitting a series of sine waves to the raw waveform and displaying the amplitude for the considered range of linear densities. Removing the harmonics, the noise power is obtained. Since the finite length of a simulated recording strip broadens the signal peak due to truncation-induced nonperiodicity, we use a special algorithm to remove artifacts in the peak width resulting from the finite bit
sequence [Renders et al., 1984]. Comparing signal statistics for the 1µm, 3µm, 9µm, and 12µm strip recordings (Table 9.1), we see that the SNR converges. The convergence with increasing strip length is due to the increased amount of transitions being included in the statistics. The artifacts due to finite length sampling are effectively eliminated [Renders et al., 1984].

Table 9.1: Signal and noise power, SNR, and jitter for 1 µm, 3 µm, 6 µm, 9 µm, and 12 µm recordings.

<table>
<thead>
<tr>
<th></th>
<th>1 µm</th>
<th>3 µm</th>
<th>6 µm</th>
<th>9 µm</th>
<th>12 µm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Signal power</td>
<td>$2.77 \times 10^7$</td>
<td>$3.05 \times 10^8$</td>
<td>$1.15 \times 10^9$</td>
<td>$2.55 \times 10^9$</td>
<td>$4.70 \times 10^9$</td>
</tr>
<tr>
<td>Noise power</td>
<td>$5.29 \times 10^6$</td>
<td>$2.50 \times 10^7$</td>
<td>$9.26 \times 10^7$</td>
<td>$1.92 \times 10^8$</td>
<td>$3.72 \times 10^8$</td>
</tr>
<tr>
<td>SNR</td>
<td>7.18 dB</td>
<td>10.86 dB</td>
<td>10.93 dB</td>
<td>11.22 dB</td>
<td>11.02 dB</td>
</tr>
<tr>
<td>Jitter</td>
<td>3.05 nm</td>
<td>1.91 nm</td>
<td>1.88 nm</td>
<td>1.90 nm</td>
<td>1.83 nm</td>
</tr>
</tbody>
</table>

Figure 9.7 shows the transition misplacement distribution. The standard deviation of the misplacement, $\sigma_{\text{jitter}}$, quantifies the jitter. Jitter is the dominant source of noise in conventional PMR. The evaluation of the jitter for a particular track is dependent on the read head model. A wider head statistically averages over a greater transition width and smoothes out the irregularities due to the granular media microstructure. The extent to which areal densities can be increased for a given microstructure by reducing either bit length or bit width closely depends on the amount of jitter noise that is introduced by the reduction of bit dimensions. Typically, $\sigma_{\text{jitter}}$ up to 10% of the bit length is tolerable.

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10 Heat Assisted Magnetic Recording

In this chapter we consider heat assisted magnetic recording as a means to extend magnetic storage capacities. Principles of operation are discussed, recent demonstrations are cited, and extendibility is addressed. A micromagnetic study is presented, illustrating that the magnetic field switching rate and the optical spot size can be used to effectively modulate the down-track and cross-track linear densities [Lomakin et al., 2011, Lubarda et al., 2011a, Lubarda et al., 2012a]. Bit patterns obtained from simulations based on modeling described in section 5.3 and chapter 7 are analyzed for signal quality, according to the procedure presented in section 9.2.4. The extent to which the signal-to-noise ratio is affected by increases in the down-track and cross-track densities is examined.

10.1 Motivation

In the previous chapter, we indicated that achieving greater areal densities in perpendicular magnetic recording (PMR) involves scaling down grains, reducing switching field distributions (SFDs), and maximizing write field gradients to obtain sharper transitions. Important tradeoffs inherent to conventional PMR which limit achievable areal densities to approximately 1 Tb/in\(^2\) were outlined. Superparamagnetism was identified as the principal problem in the effort to engineer high density magnetic recording media. Superparamagnetism reflects the magnetically unstable state of the recording medium that occurs when the grains are scaled down to volumes for which \(KV < 45k_B T\), where \(K\) is the anisotropy energy density, \(k_B\) is the Boltzmann constant, and \(T = 300K\). Under such circumstances, the magnetization of the bistable grains undergoes large fluctuations due to the influence of thermal agitation which can lead to
spontaneous reorientation, a process known as thermally activated reversal.

To avoid thermally induced erasure of stored data and yet allow for small grain volumes (necessary for high areal densities), one may consider to increase the anisotropy energy density of the media, $K$. This has been the procedure conventionally used to achieve higher areal densities in magnetic recording systems. However, the procedure is only useful up to a certain point. In section 9.1.4, it was pointed out that the unavailability of magnetic materials with $M_s > 2000 \text{ emu/cm}^3$ limits the head field amplitude $H_{\text{head}}^{\text{max}}$ to around 10–20 kOe. Since the media switching field is proportional to the anisotropy energy density, $H_{\text{sw}} \sim 2K/M_s$, increasing $K$ is efficacious only up to the limit $H_{\text{sw}} = H_{\text{head}}^{\text{max}}$.

Other tradeoffs were discussed as well. In section 9.1.3 we have indicated that improving write field gradients reduces the write field strength, which further lowers the limit on $K$ and hence grain volume, thermal stability, and signal-to-noise ratio (SNR). A new recording technique known as heat assisted magnetic recording (HAMR) was introduced to overcome these limitations by greatly relaxing the tradeoff between writability and stability, and allowing for major increases in effective recording gradients, thereby potentially deferring the upper bound on areal density by roughly two orders of magnitude.

### 10.2 Principles of Operation

Ultra-high density media requires very high anisotropy to ensure thermal stability. For areal densities beyond 1 Tb/in$^2$, the magnetic field from the write head will not be sufficient to switch bits. That is why in HAMR the recording head is equipped with a light delivery system and the media has a strong anisotropy dependence on temperature. As light locally heats the portion of the media that is to be written, media anisotropy is reduced, allowing the magnetic field from the head to write information. Since the head is constantly advancing ($\sim 20 \text{ m/s}$) relative to the media during recording, the regions of freshly written bits quickly cool off ($\sim 1 \text{ ns}$) as the thermal source moves away. Thus, the recorded magnetization is rapidly frozen in as the medium regains its high room-temperature anisotropy necessary for long-term stability.

Since the magnetic field from the write head can only record on grains at elevated temperatures, it is essential that the thermal source is placed near the pole tip. It is also important that the thermal spot size be small to ensure that the neighboring bits are not thermally agitated. Good placement of the thermal source ensures the grains are
heated just before passing beneath the pole tip. A schematic depiction of heat-assisted recording is illustrated in Fig. 10.1.

The physics of the recording process in HAMR markedly differs from that of traditional PMR. Simulation studies and recent demonstrations show that optimal HAMR performance is achieved when the grains are elevated to temperatures near the Curie point ($T_C$) or beyond. At such high temperatures, the atomic spins in the magnetic media are highly disordered and the magnetic properties of the medium are significantly altered. Atomistic simulations capture many details of the demagnetization and remagnetization processes during heating to $T_C$ and beyond, as well as during cooling back down to room temperature [Chubykalo-Fesenko et al., 2006b]. The results of atomistic simulations can enter micromagnetic models as parameterized variables. In section 5.3, we introduced the Landau-Lifshitz-Bloch (LLB) equation which includes lateral relaxation of the magnetization, and which is regarded as valid at all temperature ranges, including above $T_C$ [Garanin, 1997]. The LLB equation is used as the basis for
In addition to achieving writability at very large media anisotropy where traditional heads fail to record, HAMR also provides a pathway to modulate the effective recording profiles. Three modes of operation have been proposed, which are outlined in Fig. 10.2. In each case, a thermal source integrated with the magnetic head generates a hotspot on the media, whose specific profile defines the region of media that is writable. The magnetic pole tip, in turn, generates a magnetic field of a given profile. The overlap of the thermal and magnetic field profiles determines the region of the medium selected for switching. In Fig. 10.2a, the thermal profile extends much beyond the magnetic field profile. In this case, the features of the magnetic pole tip alone define the effective recording gradients with which transitions will be written. On the other hand, if the boundaries of the thermal and field profiles intersect as in Fig. 10.2b, both profiles contribute to the effective write gradient. Lastly, if the field profile extends beyond the thermal profile, as in Fig. 10.2c, then it is the thermal profile that defines the effective recording gradient. Since the effective recording gradients determine the achievable down-track and cross-track areal densities, combinations of thermal and field profiles are sought which result in sharpest transitions.

Illustrations in Fig. 10.2 are, however, only schematic depictions which give the general idea of the possible writing modes. It should be understood that the thermal and magnetic field profiles have a strong spatiotemporal dependence on the characteristics of the heat source and pole tip, heat diffusion in the media, motion of the head relative to the media, switching of the magnetic recording head, and possible pulsing of the heat source. In order to evaluate the sharpness of transitions in a HAMR model, it is...
necessary to know $T(r,t)$ and $H_{\text{head}}(r,t)$. While it is the spatial overlap that specifies the instantaneous region selected for writing, it is the temporal modulation of the thermal and magnetic field profiles that specify the time window during which reversal can occur for a given medium. It is anticipated that in commercialized HAMR products it will be the thermal profile which defines the transition sharpness, not the field profile (Fig. 10.2c). This is owing to the tradeoff between the field strength and field gradient affecting magnetic recording heads, as well as due to the increased risk of thermally activated reversal of adjacent bits for the case of a much extended heat spot. Considering the case where the thermal profile defines transitions, and assuming a linear relationship between critical switching field and temperature dependent media anisotropy field $H_K(T)$, we can express the effective recording gradient as [Rottmayer et al., 2006]

$$\frac{\partial H_{\text{write}}^{\text{eff}}}{\partial r} \approx \frac{dH_{\text{head}}}{dr} - \frac{\partial H_K}{\partial T} \frac{\partial T}{\partial r}. \tag{10.1}$$

The media heating (cooling) rate is given as

$$\frac{dT}{dt} = \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} \frac{dx}{dt}, \tag{10.2}$$

with $dx/dt = v$ expressing the linear velocity of the writer. Clearly, the thermal response of the media $\langle \frac{\partial H_K}{\partial t} \rangle = \langle \frac{\partial H_{\text{head}}}{\partial t} \frac{\partial T}{\partial t} \rangle$ has to be comparable to the switching rate of the head $\tau_{sw} = \langle \frac{\partial H_{\text{head}}}{\partial t} \rangle$ in order to (i) achieve data rates competitive with conventional PMA hard drives ($f_{\text{write}} \sim 40$ GHz for $v \sim 20$ m/s and $\tau_{sw} \sim 2$ ns), and (ii) to ensure rapid cooling of bits after switching so that thermal agitation does not compromise the freshly stored information. To maximize achievable data rates and increase recording reliability, pulsing of the heat source was proposed. Under this scheme, thermal equilibration rates can be an order greater than those resulting from heat source translation alone, for which $\partial T/\partial t = 0$ in (10.2). Though recent demonstrations of heat-assisted magnetic recording reported performance in the vicinity of $\sim 1$Tb/in$^2$ [Challener et al., 2009, Stipe et al., 2010, Stipe et al., 2011], the theoretical areal density limit of HAMR has been estimated to $\sim (10–100)$ Tb/in$^2$ [Kryder et al., 2008]. This brings us to the topic of the next section.

### 10.3 Extendability

Laboratory demonstrations have already provided clear indication that thermally mediated recording can overcome the limitations of traditional PMA – but to what extent? For HAMR to be considered a promising long-term solution, one that is commercially
worth pursuing despite radical alterations to the recording process which it mandates, its areal density limit should at least be an order of magnitude beyond that of the current technology. Encouragingly, theoretical estimates suggest that the fundamental limit of HAMR is on the order of 10–100 Tb/in$^2$ [McDaniel, 2005]. To assess the degree to which HAMR can practically extend magnetic storage capacity (and the pace at which it can do it), simultaneous considerations of the optical and magnetic field delivery systems comprising the hybrid recording head, modes of head operation (overshooting, microwave generation, heat source pulsing, shingle writing), the media design (structural, magnetic, thermal, and tribological properties), the interaction between the hybrid head and the media, the read and write channel architecture, as well as consideration of materials availability, feature sizes (and the semiconductor roadmap), anticipated production cost, and level of competition from alternative technologies (e.g., solid-state memory), are mandatory. The present section focuses particularly on media design and thermal energy delivery mechanisms.

10.3.1 Advanced Media Solutions

Basic Requirements

The physics of heat-assisted magnetic recording involves optical, thermodynamical, and thermomechanical effects that are absent or less sever in conventional PMR. Consideration of these effects must play an integral part in the design of HAMR-specific media solutions. The key features that will distinguish HAMR media from conventional PMR media, and the extent to which these new features will enable higher areal density recording, are now discussed.

Since HAMR is specifically intended to facilitate magnetic recording at areal densities well beyond those of conventional PMR, HAMR media must have, as its foremost attribute, a magnetic anisotropy superbly greater than that of PMR media. The magnetic anisotropy must have a strong temperature dependence to secure the long-term stability of grains at ambient temperature, while allowing grains whose temperature has been elevated by local heating to be easily written.

The third important requirement for HAMR media is a sophisticated heat sinking mechanism. This is important for two reasons, in particular. Firstly, efficient heat sinking is essential to ensure the rapid cooling of grains after thermomagnetic switching by the hybrid head. It is important that thermalization is achieved on the order of 1 ns,
otherwise thermal agitation at elevated temperatures might have time to compromise the magnetically encoded information. The thermal response time of HAMR media will play a critical role in defining operational rates in HAMR systems. An advanced heat sinking mechanism is further important to ensure that the thermal profile of the media, $T(r,t)$, reflects the sharpness of the radiative flux gradients of the heat (light) source. A state of the art light delivery system yielding an impressively small spot size will not translate to high density recording unless the lateral flow of heat within the media that leads to profile broadening is suppressed. The heat sinking mechanism of HAMR media should therefore provide maximal heat diffusion axially, and limited diffusion laterally, in order to secure high thermalization rates and large effective recording gradients for high density heat-mediated recording.

Highly focused light delivery and limited lateral heat diffusion in HAMR media are useful only if the media grain size is small enough to support the high bit densities offered by the effective recording gradients. The average grain diameter in today’s hard drives is 7–8 nm. For HAMR to defer the areal density limit well beyond that of PMR, grain diameters of 5 nm and less will be necessary. In addition to small grain size, narrow distributions of grain properties (including structural, material, and thermal properties) will be required to maintain an ample SNR at increased storage capacities.

As was mentioned in the previous section, optimal HAMR performance is expected in the vicinity of the Curie point, which suggests that $T_C$ should be sufficiently above ambient temperature to ensure clear write margins, and yet not too high to lead to thermal degradation of the medium or excessive power requirements on thermal energy delivery. Design of advanced HAMR media solutions will therefore involve careful consideration of materials going into the media layers, as well as a prudent selection of lubricants that can withstand operating conditions [Kryder et al., 2008].

**Implementation Tradeoffs and Solution Prospects**

The extendibility of HAMR technology will closely depend on the degree to which implementation tradeoffs can be resolved. We discuss two important tradeoffs touching HAMR media.

In the previous section, we listed several basic criteria HAMR media must satisfy in order to support greater areal densities, among which were high magnetic anisotropy and small grain size. However, fabricating media with 5 nm or smaller grain diameter,
while simultaneously attaining sufficiently high anisotropy to avoid superparamagnetism, is a manufacturing challenge. The processing conditions necessary to induce high magnetic anisotropy in many systems (e.g., L1$_0$-phase FePt) also lead to an unfavorable microstructure for high density recording (section 7.1), characterized by large grain sizes, wide distributions, and suboptimal intergranular exchange decoupling. Revisions of fabrication techniques will therefore be key in simultaneously achieving the desired microstructural and chemical ordering properties of HAMR media. An review of recent progress in reducing ordering temperature, increasing granular decoupling and uniformity, and achieving high magnetic anisotropy, can be found in [Kryder et al., 2008].

Patterning is an attractive approach to achieving highly structured high anisotropy HAMR media. A patterned medium has an areal density defined by the periodicity of the lithographically defined nanodots (chapter 11), and not the grain size. The granular microstructure therefore plays a less important role in determining the storage capacity of patterned media. As a consequence, patterned media offers additional optimization possibilities for HAMR [McDaniel, 2005, Matsumoto et al., 2008].

Another important issue is the compatibility of different materials systems for thermally mediated magnetic recording. To make the most of HAMR, magnetic switching must proceed near or above the Curie temperature, $T_C$. However, repetitive heating of materials systems is known to result in degradation. Sources of degradation can include structural defects due to thermal stress, migration of atomic species, deterioration of interfaces, chemical disordering, and permanent changes in material properties including thermal response [Kryder et al., 2008]. Recognizing that HAMR media will be a complex materials system composed of many different layers (including the magnetic recording layer(s), underlayer(s), heat management layer(s), capping layer(s), and lubricants), and considering that many of the traditionally recruited materials are susceptible to thermal wear or disintegration at elevated temperatures (in particular, the lubricants, which protect the media from corrosion), it becomes clear that a lower $T_C$ would imply greater availability of materials compatible with the HAMR process. Appreciable effort has gone into researching low $T_C$, high magnetic anisotropy materials. Multilayer structures such as Co/Pd (section 11.3) can be tuned to different $T_C$ through adjustments in layer thickness. Doping is another effective approach for modulating $T_C$ in alloys such as FePt. Care must be taken, however, to ensure that the approach used to reduce $T_C$ does not negatively affect magnetic properties of benefit, such as high anisotropy (for stability),
ample magnetic moment (for read back), and reduced exchange (for quality transitions).

Another approach to achieve low temperatures of operation involves exploiting phase transitions in composite systems. FeRh/FePt is an exchange coupled bilayer system in which the FeRh is antiferromagnetic at room temperature, but turns ferromagnetic above $T_N < T_C$. The phase transition, which is due to isotropic lattice expansion, results in an increased saturation magnetization and significantly reduced coercivity [Thiele et al., 2003]. Consequently, heating the FeRh/FePt creates an exchange spring system in which the softer FeRh layer helps the higher anisotropy FePt layer to switch. Successful switching was demonstrated at temperatures slightly greater than $T_N$ which was more than two times lower than $T_C \approx 500^\circ C$. Achieving suitable granular microstructure in FeRh/FePt remains a challenge. A range of other composite designs have also been proposed to reduce operating temperatures [Kryder et al., 2008]. The general idea behind these designs is to use layers of different thermal and magnetic properties in order to achieve more favorable reversal conditions.

In summary, we have discussed key challenges facing HAMR media optimization. The tradeoff between grain size and magnetic anisotropy is a great concern for continuous granular heat-assisted recording, but less so for heat-assisted recording on patterned media. Another advantage of patterning media for HAMR is that it leads to physical separation between the nanodots. Though this space is generally filled with a nonmagnetic material during the planarization process, the nonmagnetic matrix can act as a barrier to heat flow if it is of low thermal conductivity, or if phonon scattering off interfaces is high. This would ensure high confinement of the media thermal profile arising from the thermal source. Various measures to reduce operating temperatures and prevent degradation were also discussed. Considering recent advancements and trends in film fabrication and lithography, magnetic media may not be the limiting factor to HAMR.

The topic of confined light delivery is considered next.

### 10.3.2 Controlled Optical Field Delivery

The recording heads envisioned for use in HAMR are hybrid recording heads consisting of a magnetic and optical field transducer. Due to materials limitations, scaling down the magnetic transducer for increased recording resolution will result in unacceptably reduced write fields. Consequently, improvements in the effective recording gradients will have to come from improvements in the confinement of light delivered by
the optical field transducer.

Light delivery as a mechanism to store (or assist in storing) information is not a new concept originating from HAMR. Lasers have already been used extensively in optical (and magneto-optical) phase transition recording [Kryder et al., 2008]. In optical discs, storage capacity is defined by the spot size of the light. The spot size, being diffraction limited, is dependent on the laser wavelength $\lambda$ and the numerical aperture $NA$, as expressed by Sparrow’s criterion, $d = 0.51\lambda/NA$. Improving recording density by reducing $\lambda$ can only have limited practical success. Planar solid immersion lenses (PSIL) and mirrors (PSIM), which use high-refractive index solids, have been employed to increase $NA$ and achieve greater light focus [Kryder et al., 2008]. The energy from the light focusing point must then be evanescently coupled across air to the adjacent medium to prevent broadening of the projected optical spot. Such techniques have been the basis for extending near-field optical microscopy and photolithography resolution beyond the diffraction limit in air. Demonstrations of HAMR using PSIM reported areal densities of 150 Gb/in$^2$ for 488 nm laser wavelength, and 50 Gb/in$^2$ for 830 nm wavelength; see references in [Challener et al., 2009]. The expected spot size achievable with PSIM is $\sim \lambda/4$. Consequently, PSIL or PSIM alone will not be sufficient to focus laser light well enough to allow recording at areal densities expected out of HAMR.

Considerable research has focused on near-field transducers (possibly in conjunction with PSIL or PSIM) as a means to deliver light at greatest resolution [Lee et al., 2010]. Near-field transducers exploit surface plasmon resonance and the evanescent coupling of the generated high intensity near field with the highly proximal HAMR medium to transfer thermal energy over a delivery area factors smaller than what would be allowed by conventional diffraction-limited processes. Near-field transducers can take the form of apertures, such as a concentric-grooves circular aperture, or a C aperture, or can take the form of plasmonic antenna structures, such as the bowtie antenna and the dual nanowire antenna, or the beaked triangle plate, a summury of which can be found in [Kryder et al., 2008]. Different shapes and materials selections result in different plasmonic resonance excitations, an understanding of which is essential for the design of optical near-field transducers. Plasmonic materials that are commonly used for frequencies in the visible range are Ag, Au, Cu, and Al.

The interaction between the plasmonic transducer and the highly lossy metallic recording medium must be carefully considered for the optimization of confined light
delivery. A key challenge facing near-field light delivery is addressing the tradeoff between spot size and transmission efficiency. Low transmission efficiency directly implies reduced data rates due to the extended period of time required to transfer enough thermal energy to heat the medium up to $\sim T_C$.

Substantial strides have been made in enhancing optical coupling efficiency [Srituravanich et al., 2008, Sendur et al., 2005]. It was recently shown that significant near-field enhancements and coupling is possible using a gold NFT having the shape of lollipop that combines the benefits of enhanced narrow-gap resonance and the lightening rod effect [Challener et al., 2009]. The medium (FePt) response time to heating was $\sim 1$ ns, indicating strong coupling. Cross-track and down-track dimensions were $\sim 75$ nm and $\sim 35$ nm, respectively, indicating a well confined light spot. The estimated areal density of recording was $\sim 2.5$ Tb/in$^2$.

A highly integrated write head design employing an advanced metallo-dielectric laser [Mizrahi et al., 2008, Nezhad et al., 2010] has also been recently proposed [Lomakin et al., 2011]. The metal-coated laser is affixed to the main pole of the magnetic head, has a small effective footprint owing to small device dimensions and mode confinement, and exhibits low threshold gain enabling it to lase at room temperature. The light from the laser is used to drive a NFT that is integrated with the pole tip and specifically designed for highly efficient delivery of heat over an area whose overlap with the magnetic field profile can be tuned. The efficient delivery of energy is achieved though mode and plasmonic enhancement, and sharp edge localization. The produced hotspot for the modeled design was calculated to be 30 nm in size.

In summary, the progress toward ever greater light confinement continues from progress made in optical storage and microscopy. Benchmark demonstrations have shown $>2.5$ Tb/in$^2$ heat-assisted recording with a hybrid head including a PSIM light condenser combined with a NFT integrated with the magnetic writer [Challener et al., 2009]. Further gains in areal densities will depend on the extent to which the optical spot size can be reduced without compromising throughput. Considering the advancements recently made to achieve greater field enhancements, and acknowledging the breadth of the effort devoted to NFTs, not only for improving HAMR, but also for enhancing near field microscopy and photolithography resolution, and developing biosensing and DNA-sequencing techniques, it is reasonable to expect a continuation of progress which may ultimately result in high coupling efficiencies and optical spot sizes $\sim 100\times$ below the diffraction limit that can
provide the push toward heat-assisted magnetic recording at $\sim 10$ Tb/in$^2$, $\sim 20$ Tb/in$^2$, and possibly beyond.

10.4 Recording Simulations and Signal Analysis

As discussed in previous sections, the quality of the recorded bit patterns in HAMR critically depends on the magnetic field profile, switching rate of the magnetic writer, the thermal profile and heat transfer efficiency, the temporal modulation of the heat source (in case of pulsing), thermomagnetic properties of the media (e.g., temperature dependence of anisotropy, saturation magnetization, etc.), and heat diffusion in the media. In the following sections we present our preliminary exploration of some of these issues using micromagnetic simulations based on the LLB equation (section 5.3).

10.4.1 Media Model

A granular recording strip is modeled, having a cross-track width of 200 nm and down-track length of 1.5 $\mu$m. The granular microstructure of the medium is obtained from a Voronoi diagram, as described in section 7.2. We have chosen a 6 nm average diameter for the grains, and a uniform grain thickness of 10 nm. The media grains are separated from each other by roughly 0.5 nm, to account for the region occupied by the nonmagnetic segregant. The material parameters assigned to the grains resemble those

![Figure 10.3:](image-url) Normalized equilibrium magnetization (blue curve) and longitudinal and perpendicular susceptibilities (red and black curves) as a function of temperature for the L1$_0$-phase FePt system.
of ordered L1₀-phase FePt [Kazantseva et al., 2008]. This implies a $M_e(T = 0) = 400$ emu/cm³ zero-temperature equilibrium moment density, $T_C = 660$ K Curie temperature, and a temperature dependence of normalized equilibrium magnetization $m_e(T)$ and perpendicular and longitudinal susceptibilities $\chi_\perp(T)$ and $\chi_\parallel(T)$ as given in Fig. 10.3 [Bunce et al., 2010]. The coupling to the thermal bath was chosen to be $\lambda = 0.1$.

### 10.4.2 Magnetic Head Profile

The head profile used in the simulations presented here is the same as that used in the simulation of conventional perpendicular magnetic recording presented in section 9.2. Similarly as there, we consider that the writer is moving at a velocity of $v = 20$ m/s relative to the media, but we now consider two different switching periods of the magnetic head, $\tau = 2$ ns and $\tau = 1$ ns, translating to linear recording densities of 1275 and 2550 kfcic, respectively. Temporal modulation of the magnetic head profile is of the form $e^{-t/\tau}$.

### 10.4.3 Thermal Profile

We assign a temperature to each grain in the media model based on the function $T(x - vt, y)$. Here, $x$ and $y$ represent the down-track and cross-track coordinates, $t$ denotes the time, and $v = 20$ m/s is the speed of the heat source relative to the media.
We have modeled the function $T(x - vt, y)$ to simulate the heating and cooling of the media accompanying thermally assisted recording. A temperature profile $T(x - vt, y)$ with a nominal spot size of 30 nm is illustrated in Fig. 10.4. Such a hotspot is in reasonable agreement with the data produced by the recently modeled highly-integrated magneto-optical transducer, which was uniquely designed for enhanced optical field localization and controlled field delivery [Lomakin et al., 2011]. Two other thermal profiles are considered, corresponding to nominal hotspot sizes of 60 nm and 90 nm. Figure 10.5 shows the magnetic strip during heat-assisted recording using a 90 nm hotspot.

### 10.4.4 Recording Simulations

Micromagnetic simulations were used to record bits at 2 ns and 1 ns magnetic field switching rates, using hotspots of 30 nm, 60 nm, and 90 nm in size. All simulations were based on the LLB equation (5.11) [Garanin, 1997]. The computation of all relevant fields was performed according to the description provided in section 7.5. The numerical integration procedure used to evolve the dynamical equation was the Heun method. The Heun method is a suitable integrator for the stochastic LLB equation as it obeys the rules of the Stratonovich calculus (chapter 5).

Figure 10.6 shows the recordings obtained for all six combinations of switching rates and thermal profiles. The bit patterns of all six recordings can be easily discerned by naked eye, indicating robust signal. The bottommost recording in Fig. 10.6b corresponds to an areal density of $\sim 1.3$ Tb/in$^2$, assuming a 50 nm track width.
Figure 10.6: Bit patterns obtained using 90 nm, 60 nm and 30 nm hotspots for (a) 2 ns write field switching period and (b) for 1 ns write field switching period.
Figure 10.7: Readback signal amplitude (black curve, top plot) and sinusoidal fit (red curve, top plot), signal and noise power (black and red curves, bottom plot), and bit pattern (right image) for (a) 90 nm, (b) 60 nm, and (c) 30 nm hotspots using 2 ns write field switching period.
Figure 10.8: Readback signal amplitude (black curve, top plot) and sinusoidal fit (red curve, top plot), signal and noise power (black and red curves, bottom plot), and bit pattern (right image) for (a) 90 nm, (b) 60 nm, and (c) 30 nm hotspots using 1 ns write field switching period.
10.4.5 Signal Analysis

The bit patterns obtained from the simulations described above were analyzed following the procedure outlined in section 9.2. Figure 10.7a shows the signal amplitude and noise power for 1275 kfcf bit patterns recorded using a 2 ns magnetic field switching period and 90 nm, 60 nm, and 30 nm hotspots. Estimating the track widths (based on the bit widths) for the three cases to be 150 nm, 100 nm, and 50 nm, respectively, we can calculate the areal densities for the three corresponding recordings to be 230 Gb/in$^2$, 344 Gb/in$^2$, and 688 Gb/in$^2$. Signal amplitude and noise power for the same hotspot sizes, but a magnetic field switching period of 1 ns (corresponding to a 2548 kfcf linear density), are plotted in Fig. 10.8. The estimated areal densities for 90 nm, 60 nm, and 30 nm hotspots, respectively are 460 Gb/in$^2$, 688 Gb/in$^2$, and 1.37 Tb/in$^2$.

The bits obtained using a 90 nm hotspot size are similar in shape to the bits typically observed in conventional perpendicular magnetic recording. This is because for the case of a 90 nm hotspot, the magnetic field profile primarily defines the transitions, both in the down-track and cross-track directions (Fig. 10.2a). For the case of a 30 nm hotspot, the thermal profile plays a critical role in defining bit shapes (Fig. 10.2c), as reflected in Fig. 10.7c and Fig. 10.8c. In spin stand demonstrations, the quality of transitions obtained using narrow hotspots can be found significantly greater compared to the quality transitions in conventional media produced by the magnetic field alone [Rottmayer et al., 2006].

To assess the quality of recordings obtained with reduced hotspot sizes and increased switching rates, we consider the signal and noise power, SNR, and jitter. It should be noted that the value of these quantities depends not only on the bit pattern but also on read head sensitivity [Yuan and Bertram, 1994]. All the results in Fig. 10.7 were obtained using a read head sensitivity profile associated with a single read head model. A similar potential, but with the down-track $\sigma$ increased by a factor of two, was used to obtain results for the case of an increased switching rate of 1 ns (Fig. 10.8), corresponding to a linear density of 2550 kfcf, twice higher than that characterizing the bits in Fig. 10.7. It is also possible to modulate the cross-track reader sensitivity to optimize readback for narrower track widths obtained using narrower hotspots, but this was beyond the scope of the present study.

With the chosen head sensitivity potentials, we obtain for the recording pattern in Fig. 10.7a (2 ns switching, 1274 kfcf linear density, 90 nm hotspot) a signal power
of $5.16 \times 10^7$, noise power of $4.01 \times 10^6$, SNR of 11.1 dB, and jitter of 1.91 nm. For the recording in Fig. 10.7b at 1274 kfcis using a 60 nm hotspot, we get for the signal power $4.34 \times 10^7$, for the noise power $5.03 \times 10^6$, for SNR 926 dB, and for jitter 2.40 nm. For the last 1274 kfcis pattern at the narrowest 30 nm hotspot, we calculate $2.66 \times 10^7$ signal power, $6.02 \times 10^6$ noise power, 6.47 dB SNR, and 3.31 nm jitter. Using a read head potential with twice greater down-track $\sigma$, for the 2550 kfcis recording at the largest 90 nm hotspot (Fig. 10.8a), we have signal power $3.55 \times 10^6$, noise power $7.64 \times 10^5$, SNR 6.67 dB, and jitter 3.04 nm. For the same linear density but a hotspot of 60 nm, the signal power is $4.66 \times 10^6$, the noise power is $1.25 \times 10^6$, the SNR is 5.72 dB, and the jitter is 2.34 nm.

Increasing the cross-track density by using a more narrow hotspot, or increasing the linear density by increasing the magnetic field switching rate, implicates a reduction in SNR. The SNR-areal density characteristics are of critical importance in guiding efforts to extend storage capacities [Bertram and Williams, 2000]. Our preliminary study exposes the trend in declining SNR with increasing switching rates and decreasing hotspot dimensions. At 688 Gb/in$^2$, the SNR obtained from the 2 ns switching period and 60 nm hotspot recording was nearly the same as that obtained from the 1 ns switching period and 90 nm hotspot recording. Reducing the cross-track linear density is typically expected to less severely affect SNR than reducing the down-track linear density. However, the sensitivity of the read head potential used in signal calculation plays an important part in determining the SNR. More significant SNR estimates at areal densities of 1 Tb/in$^2$ and beyond (targeted densities for HAMR applications) must come from more systematic investigations involving careful consideration of read head sensitivity potentials as well as magnetic field and temperature distributions. While in this study the temperature of the media grains was prescribed based on a modeled thermal profile, explicitly including heat transfer and diffusion in our computational framework will enhance our solvers predictive power and provide for more quantitative analysis of the heat-assisted recording process. Efforts to develop such an integrated solver are ongoing.
11 Bit Patterned Media

The present chapter examines the advantages of bit patterned media for ultra-high density magnetic recording. Following an introduction, key implementation challenges are described. Proposed structural and material solutions are discussed for offsetting existing limitations. The scalability of patterned Co/Pd multilayer islands is examined. Numerical and experimental results are found to be in close agreement [Tudosa et al., 2012]. Results indicate the inherent connection between island dimensions, reversal modes, and thermal stability. A new design called capped bit patterned media, characterized by a lateral and vertical exchange, is considered for 4, 6, and 10 Tb/in$^2$ recording [Lubarda et al., 2011c]. A performance comparison is made with other bit patterned media models in terms of writability, switching field distributions, and thermal stability. Antiferromagnetic coupling between the capping layer and the patterned islands is shown to provide readback modulation [Lubarda et al., 2011b].

11.1 Introduction to Bit Patterned Media

First introduced as a steel wire in the late 1800s, magnetic recording media underwent a number of transitions, including the transition to particulate films, and more notably the transition to polycrystalline thin-film media, the latter of which has been in use for the past three decades, and has allowed information storage capacity to reach 500 Gb/in$^2$, where it stands today. Significant increases beyond this mark are difficult as the grains comprising the bits in conventional granular media have been reduced to the point where any further miniaturization would lead to thermal instability and rapid degradation of stored information (section 9.1.4). A departure from the conventional scaling routine is therefore inevitable, and may involve an updated recording scheme, such as energy assisted recording, or a transition from the continuous granular thin-film medium to a more structured storage platform. Both approaches are envisioned as likely
candidates to extend areal densities of magnetic recording beyond 1 Tb/in$^2$. The former approach was covered in detail in chapter 10. The present chapter is devoted to the latter approach, focusing on the structure of the recording medium itself.

11.1.1 Patterned Media Architecture

With continual advancements in nanofabrication technology, it was becoming apparent that patterning a continuous magnetic medium into an array of uniformly separated magnetic islands is a promising approach to defer the superparamagnetic effect and achieve superb areal densities. Bit patterned media (BPM) was first proposed in 1994 [Chou et al., 1994], with the key idea to eliminate the irregularity of continuous recording media that is inherent to its granular microstructure. This microstructural irregularity imposes the need to statistically average over a large number of grains per each bit. Since grains in conventional recording media are exchange decoupled (section 7.1), it is the volume of the grain $V_g$, not the volume of the bit $V_b$, which factors into the stability of the stored information via the expression $\Delta E_g = KV_g$, where $\Delta E_g$ denotes the energy barrier and $K$ is the anisotropy energy density. Contrary to this scheme, in BPM it is the volume of the bit (island) that determines the stability, $\Delta E_b = KV_b$. This is because each island consists of a single grain, or is composed of several grains that are strongly exchange coupled. Since the patterned islands are magnetically isolated and uniformly spaced, a bit volume much greater than the grain volume used in conventional media can be used to achieve the same areal density. This point is illustrated in Fig. 11.1, which demonstrates that BPM can offer thermally stable recording at areal densities where conventional continuous media is superparamagnetic.

Other advantages in the recording and storage performance of BPM in comparison with continuous granular media include: improved signal-to-noise ratio (SNR) and reduced dipolar coupling between bits, both on account of the physical spacing between the patterned islands; greater stability and writability, afforded by the greater thermal activation volume and the possibility to reduce $K$ without entering the superparamagnetic regime; greater homogeneity due to islands being comprised of a single grain or consisting of several grains strongly exchange coupled; greater adaptability to heat assisted magnetic recording (HAMR, chapter 10) because of the physical separation of the islands which can be surrounded by a low heat conductivity matrix that limits how much heat can dissipate from the thermally targeted region to the surrounding bits. The encouraging list
of advantages indicates that BPM can be pushed to areal densities far beyond those that could possibly be supported by traditional continuous recording. Nevertheless, realization of magnetic recording on ultra-high density BPM will require further advancements in nanofabrication technology to achieve the needed patterning fidelity and throughput, and additional improvements in systems engineering for overcoming the difficulties inherent to recording at 1 Tb/in$^2$ and beyond.

### 11.1.2 Implementation Challenges

Despite recent laboratory demonstrations of magnetic recording on BPM at 1 Tb/in$^2$ (e.g., see [Stipe et al., 2010]), there still remain a number of challenges facing the commercialization of bit patterned disk drives. One of the challenges is the high cost and low throughput of the BPM fabrication process [Terris, 2009]. Electron beam
lithography is both expensive, due to vacuum ambient requirements, and slow, due to a single beam writing source. Moreover, the beam spot size is inversely proportional to the patterning time, placing a severe tradeoff between areal density and throughput. Of the patterning techniques considered for BPM, nanoimprinting lithography comes closest to meeting the manufacturing yield requirements and the low cost necessary for mass production. Master molds need be created only once, using electron beam lithography or self-assembly, following which, replicas of the master stampers may be produced, and used for large-scale BPM fabrication.

Pattern fidelity is another key concern. Analyses show that the distributions in island position, size, and shape, distinctly affect recording performance. For reliable recording on BPM, these distributions must be under 10% [Sbiaa and Piramanayagam, 2007, Schabes, 2008, Thomson and Terris, 2012]. Current accomplishments in patterning in excess of 1 Tbit/in² exceed the quoted distribution width in terms of island placement and size distributions. Considerable improvements are necessary to achieve the necessary uniformity for first generation BPM disk drives.

Commitment to full system integration and production will come once it becomes convincingly clear that the extendibility of magnetic recording on BPM is sufficiently great to meet the demands of the consumer market in the years to come. This means that the transition to BPM will not only be contingent on optimizing the fabrication process to deliver high fidelity patterned media at 1 or 2 Tbit/in², but also on the prospect of meeting the technological challenges associated with additional increases in areal density to 5 Tbit/in², 10 Tbit/in², and possibly beyond, at a pace proportional to the rate of development of emerging applications and the continuing growth in high-capacity storage requirements.

Considering that several competing technologies are equally under development, and that the areal density projections obtained from Moore’s law for magnetic recording over the next two decades translate to BPM feature sizes that surpass what is expected to be lithographically achievable based on the semiconductor industry roadmap, timelines for BPM implementation cannot be quoted with certainty. To what extent might energy assisted recording or solid-state memory in a timely manner accommodate the storage needs of tomorrow, is equally questionable, as both face a series of challenges of their own. The amount to which future devices will be dependent on local storage will have an additional bearing on the pace of development of ultrahigh areal density media.
Though the rate at which recording areal densities increase may fall in the short-term due to the number of immediate challenges outlined above, it can nonetheless be expected that increases in recording capacity will eventually regain pace once a certain technological threshold is reached. This is likely to happen after the first round of energy delivery and materials challenges facing heat assisted recording are met, and after patterning techniques are perfected, at which point areal densities as high as 20 Tbit/in$^2$ may be within reach.

We have mentioned extrinsic distributions in island position, size, and shape to be a serious challenge associated with the BPM fabrication process. Another outstanding challenge is reducing intrinsic distributions of the magnetic properties of the islands. This includes fluctuations in easy axis direction, anisotropy energy density, saturation magnetization, exchange energy density, and damping. Such fluctuations cause additional distributions in switching fields, thermal stability, and switching rates that deteriorate the recording and storage performance. More than anything, this is a materials problem, which requires materials solutions, a few of which are discussed in sections 11.2.3, 11.2.4, and 11.2.5. Another source of distributions comes from the magnetostatic coupling between the bits, a topic covered in sections 11.2.8, 11.4 and 11.5. Lastly, a number of system integration challenges exist, such as accommodating the recording process to the variation in the island frequency over the radius of the disk as it rotates, attaining servocontrol, maintaining head-media synchronization, ensuring ample readback signal, achieving quality planarization and ensuring good head flyability, and preventing contamination and wear. All of these challenges must be met in order to allow reliable and high-performance operation of magnetic recording on BPM.

11.2 Design Considerations for Bit Patterned Media

As with all prospective technologies, the specific design solution has a significant bearing on both implementation feasibility and overall product performance. In this section we review some of the important aspects of different BPM designs that have been proposed over the recent years.

11.2.1 Rectangular vs. Elliptical Islands

The shape of the islands is an important consideration in the optimization of the recording performance on BPM. The most common island shapes that have been
considered are of rectangular or elliptical cross-sections. Islands of aspect ratio (IAR) 1:1 have been considered, which have square or circular cross-sections, as in Fig. 11.2a or 11.2d. Islands with substantially greater IAR, such as 1:4 (Fig. 11.2b or 11.2c), have been considered, as well [Schabes, 2008]. The proximity of the islands in the down-track and cross-track directions defines the bit aspect ratio (BAR), and can be different from the IAR. It has been demonstrated that ultrahigh areal density BPM with either rectangular or elliptic islands can be obtained for a wide range of aspect ratios.

The island shapes, the IAR, and the BAR have important implications for the design of magnetic recording heads and read heads. For a BPM design at 1 Tb/in$^2$ with BAR equal to 1:1, the recording pole tip would have to be very small to accommodate for the narrow track width. Since reducing the size of the pole tip diminishes the write field output (section 9.1.3), a 1:1 BAR can result in reduced writing capability. Since the BAR in conventional perpendicular magnetic recording on continuous granular media is approximately 1:5, it may be advantageous in the short term to use a similar aspect ratio for the first generation BPM, in order to enable a smoother transition between the two media platforms [Schabes, 2008]. Considerations of IAR and BAR, and their effect on synchronization, energy delivery, heat diffusion, and bit error rates are also important in the design of heat-assisted recording on BPM [Xu et al., 2009, Greaves et al., 2011]. It

Figure 11.2: Types of patterned media arrays: (a) rectangular lattice and square islands; (b) rectangular lattice and rectangular islands; (c) rectangular lattice and elliptical islands; (d) hexagonal lattice and circular islands.
is generally agreed that a 1:1 IAR and BAR will be ultimately preferable, as this will allow for greatest storage capacity due to maximized island packing and the fact that the greatest patterning quality is expected for islands of circular geometry.

One solution that has been proposed to address the problem of writing on narrow tracks is to use an asymmetric or skewed pole tip that is much wider than a single track [Kasiraj and Williams, 2005]. The approach is known as shingled writing. In this scheme, recording extends over several tracks, with tracks written sequentially.

The shape of the islands, together with the IAR and BAR, must also be considered when accounting for dipolar coupling between bits, readback, servocontrol, head-media synchronization, and cross-track/down-track misregistration margins. Much work has already been devoted to investigating these issues [Albrecht et al., 2002, Moser et al., 2007, Lomakin et al., 2007, Schabes, 2008, Livshitz et al., 2009b, Livshitz et al., 2009a, Lubarda et al., 2011c, Ruiz et al., 2011]. Another important feature of BPM is the particular arrangement of the islands in the array, which is covered next.

11.2.2 Staggered Bit Patterned Media

So far, the shape of the islands, the IAR, and the BAR have been discussed, but nothing has been said on the particular arrangement of the islands in the patterned array. The islands in Figs. 11.2a-c were all arranged on a rectangular lattice. A hexagonal array of islands is shown in Fig. 11.2d. Such a configuration is known as staggered BPM [Richter et al., 2007]. Conceptually, the hexagonal array can be obtained from a rectangular array by simply shifting every other row by half the lattice spacing. Hence, the packing densities of rectangular and hexagonal island arrays are identical. The primary benefit of staggered BPM is reduced risk of adjacent-track bit errors [Livshitz et al., 2009b]. The lower chance of recording unintentionally on an adjacent track is owed to the fact that in staggered BPM, islands in adjacent tracks are out of phase. Such an arrangement allows for greater lateral write margins than would be possible with BPM having a rectangular lattice. A staggered arrangement is considered to be the preferred solution for heat-assisted recording on BPM, as well. Staggered BPM has also been considered as a means of achieving reduced dipolar interactions between bits. It has been recently reported, however, that for typical IAR and BAR, a hexagonal arrangement can in fact lead to greater dipolar coupling and broader switching field distributions in comparison to the rectangular case [Ranjbar et al., 2011].
11.2.3 Inclined Anisotropy Bit Patterned Media

Magnetic media with an easy axis tilted from the vertical direction by some angle $\theta_k$ has been proposed to reduce the field required to write bits, thus allowing higher anisotropy media supporting greater areal densities to be used [Gao and Bertram, 2002]. The critical write field for the case of inclined anisotropy media is also less sensitive to fluctuations in easy axis direction. Both benefits can be understood from a look at the Stoner-Wohlfarth astroid [Stoner and Wohlfarth, 1948]. It was further shown that greater switching rates can be achieved using inclined media owing to a rapid reversal process [Zou et al., 2003].

Another benefit of inclined anisotropy BPM is that the dipolar broadening of the switching field distribution (SFD) is suppressed [Honda et al., 2011]. To understand why this is so, consider an array of three islands with longitudinal anisotropy. The magnetostatic energy is minimized when the moments of the three islands are aligned in parallel, a configuration symbolically represented as $\rightarrow\rightarrow\rightarrow$. Conversely, for a three-island array with perpendicular anisotropy, the magnetostatic energy is minimized when the magnetization configuration is antiparallel, $\otimes\circ\otimes$. Since inclined anisotropy BPM is a compromise between the longitudinal and perpendicular orientations, the favorability toward the parallel or antiparallel configuration is appreciably neutralized. For a two-dimensional island array, the magnetostatic interplay between the islands is more complicated, but a net reduction in the SFD is still achieved.

Two important challenges in the implementation of inclined anisotropy BPM are fabrication and readback optimization.

11.2.4 Exchange Coupled Composite Bit Patterned Media

It has been observed that the switching field of a bilayer system, where a soft magnetic layer is coupled to a magnetically hard layer (Fig. 11.3a), is much lower than the switching field of the hard layer alone [Fullerton et al., 1998]. The reduced switching field is due to the fact that, upon an applied field, the magnetization of the soft layer is the first to begin to reorient, by which action it exerts an additional torque on the hard layer, thus helping it reverse (Fig. 11.3b) [Suess et al., 2005, Victora and Shen, 2005a]. The new reversal mode additionally reduces sensitivity to fluctuations in anisotropy [Victora and Shen, 2005b]. It was further shown that the thermal stability of a soft/hard bilayer is no less than that of the hard layer alone, despite the reduction in the switching field [Suess
et al., 2005]. The exchange coupled composite (ECC) design has already been employed in perpendicular magnetic recording on continuous granular media and can be extended to BPM. Besides the reduced switching fields at constant thermal stability, ECC BPM has also been shown to allow for reversal in the precessional regime, which leads to an additional reduction in switching fields [Livshitz et al., 2007]. The criteria for precessional reversal, which for the case of single-layer BPM include ultra-short field rise times, are relaxed by an order of magnitude for ECC BPM. It has also been demonstrated that for ECC BPM the necessary microwave frequency required for microwave-assisted reversal is significantly lower than for single-layer BPM [Li et al., 2009b].

11.2.5 Islands with Multiple Magnetic Layers

For many purposes it is advantageous to have the patterned islands consist of many magnetic layers of different materials or compositions. It has been shown that graded media, where each subsequent layer is lower in anisotropy from the previous (Fig. 11.4), results in a dramatic reduction of the switching field, while still preserving the needed thermal stability [Goncharov et al., 2007, Suess et al., 2005]. For an optimal anisotropy gradient, magnetization reversal can occur in principle at arbitrarily low fields. Multiple layers of different materials can also be used to reduce intrinsic SFDs [Krone et al., 2010]. Since variations in material properties often propagate vertically across a single layer, such as deviations in easy-axis direction due to stacking faults, it can be helpful to have several different layers to decorrelate these variations, and thus achieve a lower net variation...
Figure 11.4: Graded anisotropy island consisting of multiple magnetic layers of increasing anisotropy.

within each island. A \([\text{Co/Pd}]_N \text{Fe}[\text{Co/Pd}]_{N'}\) trilayer design has recently been shown to simultaneously reduce the switching field, SFD, as well as the resonance frequency, while maintaining the high anisotropy necessary for thermal stability [Eibagi et al., 2011]. Since the resonance frequency is typically positively correlated with the anisotropy, the decoupling of the two, as achieved in \([\text{Co/Pd}]_N \text{Fe}[\text{Co/Pd}]_{N'}\), is paramount for high density microwave assisted magnetic recording.

11.2.6 Three Dimensional Bit Patterned Media

The use of multiple layers with different magnetic properties has been proposed for achieving three-dimensional recording or multilevel storage [Albrecht et al., 2005, Khizroev et al., 2006]. Several design proposals exist, each necessitating a new recording scheme. In one design, the thermally stable layers have markedly different anisotropy fields (Fig. 11.5). The softest layer can be addressed by an applied field that is sufficiently ample to reverse its magnetization, but weak enough not to affect the stored information in the remaining layers. Recording on the hardest layer, however, requires all softer layers to be rewritten sequentially. The disadvantage of this design is that conventional recording
Figure 11.5: Island composed of three exchange decoupled layers proposed for three-dimensional magnetic recording.

heads produce a write field of a fixed strength, whereas a multi-strength recording head would significantly complicate implementation.

A more promising three-dimensional BPM design involves microwave-assisted magnetization reversal [Winkler et al., 2009]. In this design each layer is tuned to have a distinct resonance frequency. The conventional recording head is equipped with a microwave source, which can operate at a range of frequencies. The strength of the recording head field is insufficient to record any of the layers by itself, but together with the microwave field is able to switch the particular layer whose resonance frequency matches that of the microwave source. A current-tunable microwave source with operating frequencies in the relevant range would be a spin-torque nanooscillator (section 12.1.4).

The media used for such a recording scheme can be extended to take advantage of the reduced switching fields and lower resonance frequencies achieved by ECC elements [Li et al., 2009b]. Such a media design would consist of two or more vertically stacked exchange decoupled ECC bilayers with sufficiently differing resonant frequencies (Fig. 11.6) [Kovacs et al., 2010].

An important challenge for the implementation of three dimensional storage is readback. In current state-of-the-art hard drives, the read head flies at approximately
Figure 11.6: Island consisting of an exchange decoupled pair of hard/soft bilayers having differing resonant frequencies proposed for two-level microwave-assisted magnetic recording.

an elevation of 5 nm over the media. In a three dimensional media the read head would necessarily be at an increased separation from the bottom layers, which would inevitably compromise readback resolution.

11.2.7 Ledge Bit Patterned Media

Ledge BPM consists of an array of dual-layer patterned islands, in which the magnetically soft layer has a greater cross-sectional area than the hard layer, and hence extends laterally farther (Fig. 11.7) [Lomakin et al., 2008a, Lomakin et al., 2008b]. Such ledge elements, similarly to ECC elements, are characterized by reduced switching fields and allow precessional reversal to occur at much longer field rise times than would be possible for single-layer elements. The key features that distinguish ledge BPM from ECC BPM, in terms of performance, is that the ledge elements, due to their unique geometry, can afford longer soft layers, while preserving low media thickness, as illustrated in Figs. 11.7a-c. Thin media is important to take advantage of strong write fields and sharp field gradients important for high density recording, while sufficiently long soft layers
are beneficial to allow domain wall nucleation and injection for optimal reduction in switching fields. Different arrangements of ledge elements are possible (Fig. 11.7d-f). Fabrication of ledge BPM may be more involved due to the different cross-sectional areas of the two layers.

11.2.8 Capped Bit Patterned Media

The most conspicuous feature that distinguishes BPM from traditional continuous media is that the bits are magnetically isolated. However, for purposes of recording optimization, it can be beneficial to moderately exchange couple neighboring magnetic islands. The idea is similar in many ways to modulated intergranular exchange in conventional granular media or coupled granular/continuous (CGC) media [Sonobe et al., 2001]. One advantage of the modulated interbit exchange coupling is reduced switching field distributions (SFDs). Capped BPM, where an array of patterned islands is coupled to a continuous magnetic capping layer, as illustrated in Fig. 11.8, is the most natural way to achieve the desired inter-island exchange coupling in patterned media [Li et al., 2009a, Albrecht and Schabes, 2009]. Capped BPM is characterized by both vertical and lateral exchange. It has been demonstrated that the capped BPM design enjoys several other advantages besides reduced SFDs. These include improved writability, greater thermal stability, and modulated readback response [Li et al., 2009a, Lubarda et al.,...]

Figure 11.7: Dual-layer ledge elements allowing domain wall-assisted recording at low media thickness. Possible (a)–(c) element designs and (d)–(f) array configurations.
11.2.9 Planar Bit Patterned Media

Though BPM has not been yet commercialized, the mainstream fabrication techniques used to pattern the media for purposes of characterization and study have involved the physical removal of magnetic material (milling) to achieve magnetic isolation of the bits. The resulting arrays of patterned islands require planarization and coating in order to ensure head flyability, and prevent oxidation and wear. The etching process unavoidably introduces some degree of damage, i.e., changes in the magnetic properties of the islands. Redeposition of magnetic material during patterning presents another concern. An alternative fabrication technique that does away with the milling and planarization processes is known as ion-irradiation patterning [Chappert et al., 1998]. In this technique, ions bombarded the magnetic film, and are implanted in exposed regions, where they change the magnetic properties of the material. The ion species is chosen with the aim to quench the magnetization in the exposed regions and reduce or eliminate exchange coupling between the areas unexposed. Typically, He\(^{+}\), B\(^{+}\), or Ar\(^{+}\) are used. Generally, the heavier the ion, the greater is the patterning resolution. A planar BPM analogue of capped BPM can in principle be fabricated with modulated vertical and lateral exchange.
11.3 Multilayer Nanopillars: Reversal Modes and Thermal Stability

Several promising magnetic nanotechnologies are being presently investigated in a broad effort to improve and reform the way computers, and a range of other electronic devices, store, retrieve, process, and relay information during operation. Nanotechnologies that have attracted great research interest include magnetic recording on bit patterned media, magnetic random access memory (MRAM; section 12.1.2), spin valve logic (section 12.1.3), and spin-torque nanooscillators (section 12.1.4). All have in common that their architectures include lithographically defined nanosize magnetic elements, generally referred to as nanodots, nanoislands, or nanopillars. Most commonly explored nanopillars have been multilayer nanopillars, consisting of a plurality of ultra-thin (several monolayers thick) magnetic layers separated by nonmagnetic spacer layers. Such a configuration, when properly tailored, results in perpendicular magnetic anisotropy (PMA) and provides great tunability of magnetic properties, such as the Curie temperature, and lateral and vertical exchange (section 11.2.8), through modulation of spacer layer thickness and material composition. Understanding the various types of reversal modes in magnetic multilayer nanopillars is essential for acquiring the needed insight for the design and development of thermally stable ultra-high density memories, advanced nonvolatile logic

Figure 11.9: Patterned Co/Pd multilayer island having 30–40 nm diameter with $N$ cobalt repetitions.
circuits, as well as high-performance current-tunable nanoscale microwave oscillators for telecommunication and other functions.

In many recent experimental investigations [Tudosa et al., 2012, Bedau et al., 2010b, Sato et al., 2011, Gajek et al., 2012], the extracted energy barriers separating the two bistable states of PMA nanopillars in the 30–50 nm diameter range was far below the expected energy barriers calculated as the product of the effective anisotropy and particle volume (macrospin approximation). That is, the actual nanopillar thermal stability was well below the anticipated stability in the experiments. These results have suggested an incoherent mode of reversal and a thermal activation volume less than the physical volume of the nanopillars. We first consider the findings of our experimental study of patterned $[\text{Co}(0.3 \text{ nm})/\text{Pd}(0.7 \text{ nm})]_N$ multilayer islands.

### 11.3.1 Co/Pd Multilayers: Experimental Results

Figure 11.9 is an illustration of a patterned Co/Pd multilayer island, showing an arbitrary number of Co layers separated by Pd layers. An array of such islands was fabricated first by growing the magnetic layers by DC magnetron sputtering. A self-assembling diblock copolymer solution was spin-coated onto this film to obtain a pattern. A spin-on glass pattern was ultimately used as an etch mask for the islands. After Ar ion milling, the resulting islands had the diameter in the range of 35–40 nm and a pitch of 65 nm.

Electron microscope images showing arrays of patterned Co/Pd islands with 11 repetitions obtained for etching times of 20 and 40 seconds are shown in Fig. 11.10. Islands with 3, 5, and 8 repetitions were also fabricated. If etching time is long enough,
the islands are over-etched and the island morphology is altered, as can be seen in Fig. 11.10b corresponding to the 40” etch. Conversely, if the etch is too short, not all layers may be etched all the way through, and the islands might remain laterally exchange coupled. An under-etch can therefore be used to fabricate capped bit patterned media (CBPM), the media covered in chapter 11.4. Figure 11.10a shows islands obtained for a 20” etch, where a thin layer near the base of the islands has not been etched all the way through, and so physically connects the islands. However, the layer is Ta which is nonmagnetic. Therefore, the islands are not ferromagnetically exchange coupled, which is also evidenced by the results obtained using the $\Delta H(M,\Delta M)$ method which show that the total switching field distribution ($\sigma_{\text{tot}}$) is greater than the intrinsic distribution ($\sigma_{\text{int}}$) without interaction contributions, and hence the dominant interaction type is dipolar.

Table 11.1 summarizes important properties of patterned $[\text{Co/Pd}]_N$ multilayer islands obtained for $N = 3, 5, 8, \text{and } 11$. The energy barrier between the two bistable states of the multilayer islands can be estimated from a simple macrospin calculation by multiplying the effective anisotropy energy density with the island volume to get $E_b = KV = 225 k_B T$ for $N = 3$, and $E_b = KV = 1115 k_B T$ for $N = 11$. Experimentally, the energy barriers can be extracted from the dependence of coercivity on field sweep rate, using the Sharrock formula (section 2.1.9)

$$H_C = H_0 \left[1 - \frac{1}{a} \ln \left(\frac{f_0 H_0}{2a} \frac{1}{R}\right)\right],$$  \hspace{1cm} (11.1)

where $H_C$ is the coercivity at sweep rate $R$, $H_0$ is the short time coercivity (for $R \to \infty$),

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<th>$N = 3$</th>
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<td>10.4</td>
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<td>$H_0$ (kOe)</td>
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<td>12.6</td>
<td>11.9</td>
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<td>7.3%</td>
<td>8.1%</td>
<td>7.9%</td>
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<td>$a$</td>
<td>80</td>
<td>110</td>
<td>230</td>
<td>360</td>
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Figure 11.11: Energy barrier associated with island reversal as a function of the number of Co repetitions obtained analytically using a macrospin model (red curve), micromagnetically using the nudge elastic band method (black curve), and experimentally (green curve).

\[ f_0 \text{ is the attempt frequency (} \sim 10^{10} \text{ Hz)} \text{ and } a = \frac{E_b}{(k_B T)}. \]  

Table 11.1 lists the energy barriers \( E_b \) for \( N = 3, 5, 8, \) and 11, extracted from a fit to Sharrock’s equation.

Figure 11.11 shows a plot of the expected energy barriers obtained from the macrospin calculation and the energy barrier values extracted from a measurement data for different numbers of repetitions. Clearly, there is a great discrepancy between the two curves. The expected and measured values for a multilayer with \( N = 11 \) repetitions differ by a factor \( \sim 3 \). The actual stability of the multilayer islands is therefore significantly below the anticipated value. This suggests an incoherent thermal reversal mode characterized by nucleation and DW propagation. The linearity of the energy barriers with the number of repetitions indicates that the interlayer coupling of the studied samples was in the strong coupling limit, which further implies that the domain wall (DW) motion during thermal reversal was in the lateral direction. These modes are numerically and analytically investigated in detail in subsequent sections.
11.3.2 Comparison with Spin Valves having Co/Ni Free Layer

We briefly cite another recent experiment that led to similar conclusions in regard to thermal stability and reversal modes. In [Bedau et al., 2010b], an all-magnetic spin valve nanopillar with a $[\text{Co/Pt}]_4[\text{Co/Ni}]_2$ reference layer and a $[\text{Co/Ni}]_2$ free layer was studied. Current pulses of controlled amplitude and duration were sent through the nanopillar to effect switching between the parallel and antiparallel states. Repeated measurements were performed to obtain the necessary statistics related to the switching. Two switching regimes were observed. For short pulse durations below 10 ns, the pulse amplitude was inversely proportional to the pulse duration (for 50% switching probability), coinciding with the macrospin model for current-activated reversal. For long pulse durations, the results of the experiment coincided with the analytical model corresponding to reversal activated by thermal fluctuations in the presence of spin transfer torque. Similarly, the switching probability versus pulse duration was obtained for the current-activated and thermally activated regimes. The energy barrier obtained from the fit of the analytical equations to the data for both regimes was $63 k_B T$. This was again several times below the expected value given as the product of anisotropy and volume. Therefore, while the macrospin model gives correct relationships between the relevant parameters, it does not accurately represent the energy barrier, whose value under the single-domain assumption, which was the premise of the model, was significantly larger than what was extracted from the fit of the same model. This implies, as do results of the Co/Pd multilayer study, incoherent reversal, characterized by nucleation and propagation of DWs in the structure.

11.3.3 Co/Pd Multilayer Islands: Micromagnetic Modeling

Having provided sufficient motivation for investigating energy barriers and stability of these structures beyond the single-domain approximation, we proceed to present results of micromagnetic modeling and simulations. We studied micromagnetically the stability of Co/Pd multilayer islands as a function of the number of repetitions, islands diameter, and interlayer coupling strength. Because the coupling between successive Co layers is not direct exchange, but rather coupling modulated by the Pd spacer layers, we expect different modes of reversal and stability for different strengths of lateral and vertical exchange.
Calculation of Effective Anisotropy

We wish to compare numerical calculations with the expected values obtained as the product of effective anisotropy and island volume. The insert on the right of Fig. 11.12 shows that we have computed the effective anisotropy as the energy difference between the out-of-plane and in-plane configurations of the island. The in-plane configuration is obtained by forcing the moments away from the uniaxial easy axis to point parallel to the plane of the layers. The plot to the left indicates the effective anisotropy for different number of repetitions. The effective anisotropy is most sensitive for a low number of repetitions, because in this region the in-plane shape anisotropy is most variable. The effective anisotropy was also calculated as a function of particle diameter.

Thermal Stability versus Number of Repetitions

Displayed in Fig. 11.11 is the dependance of the energy barrier with the number of repetitions. The blue line is the expected energy barrier estimated as the product of the effective anisotropy, shown in Fig. 11.12, and island volume. The red and black lines in Fig. 11.11 are the energy barriers obtained by the nudged elastic band method.
Figure 11.13: Energy barrier associated with island reversal as a function of island diameter obtained for an island with 5 cobalt layers using a macrospin model (red curve) and the nudge elastic band method (black curve).

(NEBM, section 6.2) for strong and weak interlayer coupling, respectively. Plotted green is the data obtained from experimental measurements, shown earlier. It can be seen that the experimental data and numerical calculations are in good agreement. However, the expected energy barriers, and hence the expected stability is much greater than what was obtained experimentally and numerically, implying incoherent thermal reversal of the islands accompanied by DW motion.

**Thermal Stability versus Islands Diameter**

The NEB method was also employed to calculate the energy barrier as a function of island diameter. For large island diameters the computed energy barriers are still significantly beneath the expected value. However, when the diameter is reduced, and the island approaches the Stoner-Wohlfarth limit, the thermal stability calculated micro-magnetically, plotted red in Fig. 11.13, coincides with the expected stability assuming
coherent reversal of a single domain particle. That is, as the island diameter is reduced to a size expected for patterned media applications, the discrepancy between the expected and actual energy barriers vanishes, and the full volume stability is recovered.

**Thermal Stability versus Interlayer Coupling Strength**

Lastly, before taking a closer look into the modes of thermal reversal, we consider the dependance of the thermal energy barrier on interlayer coupling strength. The coupling strength is tuned experimentally by changing the thickness of the Pd spacer layer in the multilayers. Computationally this is done simply by varying the value of interlayer exchange energy. The plot in Fig. 11.14 shows the energy barrier increasing with coupling strength until saturation. This calculation was performed for a multilayer with three Co layers. At zero interlayer coupling, as expected, the stability of the multilayer is very nearly equal to that of a single layer of Co. (The slight difference is due to the influence of the demagnetization field.) At saturation, when interlayer coupling is sufficiently large, the energy barrier is closely equal to three times the value of a single layer of Co, which is expected, because the multilayer in this example consists of three repetitions. Saturation, here, implies vertical coherence under thermal reversal, but does not restrict lateral DW motion. In fact, we inferred from experimental results on the dependence of energy barriers on the number of repetitions that lateral DW motion is the mode of reversal for the fabricated islands, which means the islands were in the strong coupling limit.

**Thermal Reversal along the Minimum Energy Path**

Figure 11.15a gives an outline of the thermal reversal for a multilayer with strong interlayer coupling showing the magnetization configuration of the island at different points along the minimum energy path obtained by the NEB method. At the far left we have the island in its initial state, oriented upward, perpendicular to the plane of the layers. A DW nucleates at the island edge, across all layers, with full vertical coherence due to large interlayer exchange, and then the DW grows, propagating along the island. The configuration of greatest energy occurs when the DW size is at its maximum value. Beyond this point, the energy decreases as the DW reduces in size, and eventually exits the particle, leaving it in its reversed state.

For weak interlayer coupling, the reversal process is more diverse, and can be
accompanied by several energy barriers (Fig. 11.15b). In this diagram, a DW nucleates initially at the bottom layer only, after which it laterally propagates, reversing the bottom layer, and leaving the island in an intermediate metastable state (Fig. 11.15b). The energy at this location is higher than the energy of the initial state due to the creation of a vertical DW situated between the first and second layer. Next, the middle layer nucleates, also at the edge, wherefrom the DW grows, and the energy increases, after which the DW shrinks and exits. The top layer follows suit, ultimately leaving the island fully reversed. The energy of the final and initial state for the single island is, of course, the same.
Figure 11.15: Reversal along the minimum energy path for Co/Pd island having three (a) strongly exchange coupled and (b) weakly exchange coupled cobalt layers.
Figure 11.16: Analytical model of thermal reversal for a Co/Pd/Co system showing energy paths for vertically coherent and vertically incoherent reversal for (a) strong, (b) moderate, and (c) weak interlayer coupling.

Comparison to Analytical Model

We have also looked at the thermal reversal predicted by an analytical model. Figure 11.16 shows a simple two layer system. Two possible modes of thermal reversal are assumed: layer-by-layer switching, as occurring for weak interalayer coupling (Fig. 11.15), and vertically coherent reversal, where the DW nucleates simultaneously across all layers and propagates laterally, as shown in Fig. 11.15a for the case of strong interlayer coupling. Taking into account the energy of the lateral and intralayer DW, and the magnetostatic energy (see equation chart in Fig. 11.16), one analytically obtains energy paths (Fig. 11.16) in close agreement to ones obtained using the NEBM (Fig. 11.15). The plots show the energy as the island reverses for different values of interlayer coupling strength. The red and blue colors correspond to vertically coherent and layer-by-layer reversal, respectively. For large interlayer coupling, the energy path with the lower energy...
barrier is that of the vertically coherent reversal mode, as seen in Fig. 11.16a. Indeed, with large interlayer coupling, the energy expense of placing a DW between layers is much too great. For intermediate interlayer coupling, shown in Fig. 11.16b, the energy barriers for the vertically coherent and incoherent modes are similar. Lastly, for weak interlayer coupling, the vertically incoherent mode corresponding to layer-by-layer switching is the preferred mode of thermal reversal, having the lower energy barrier (Fig. 11.16c). This trend is the same as that shown in Fig. 11.15 for the trilayer island, whose energy paths for different interlayer coupling strengths were obtained numerically.

11.3.4 Summary and Outlook

In summary, the presented micromagnetic study was motivated by stability measurements of perpendicular anisotropy devices, more specifically, multilayer islands and spin-valve nanopillars, the stability of which is crucial for bit patterned media and anticipated STT applications. We have observed the inherent connection between DW configurations, modes of propagation, and thermal stability. We have micromagnetically modeled Co/Pd multilayers and numerically studied their stability as a function of the number of repetitions, island diameter, and interlayer coupling strength. The calculated energy barriers were in good agreement with experimental results, but the stability was several times less than the expected value. The mode of thermal reversal obtained by the NEBM revealed that reversal is indeed not coherent, as indicated by the energy barriers found experimentally. In the Stoner-Wolhfarth limit, valid for reduced island diameters, we found that the numerically computed and expected energy barriers do coincide, i.e., the full volume anisotropy enters the island stability, and the reversal in this case is coherent. Further, we found that modulating the lateral and vertical exchange in the multilayer systems allowed us to transition between the different modes of reversal. In the strong coupling limit, DWs nucleate across all layers simultaneously and propagate with full vertical coherence, while for reduced interlayer coupling, layer-by-layer switching prevails and the thermal stability is lower.

Future work will include developing a more comprehensive understanding of the influence of externally applied fields and spin currents on the stability and DW configurations in magnetic nanostructures. This will be important for novel spin-based applications, particularly in light of the recent observations of the existence of intermediate stable states in similar nanostructures to the ones studied here, which were shown to be
Figure 11.17: Bit patterned media designs: (a) homogeneous BPM (HBPM); (b) exchange coupled composite (ECC) BPM; (c) ledge BPM; (d) capped BPM (CBPM); (e) composite capped BPM (CCBPM).

sustainable only under the joint influence of applied fields and spin currents [Cucchiara et al., 2009]. These new stable states correspond to DWs residing at specific pinning sites in the nanopillars. Dwell times and transition rates were shown to be controllable by external fields and spin currents. Understanding DW processes activated by thermal fluctuations under spin transfer torque will not only be important for ensuring reliable operation of MRAM, but also for developing novel STT-based applications with new functionalities.

Acknowledgements: Section 11.3 in Chapter 11 is based on the journal article: I. Tudosa, M. V. Lubarda, K. T. Chan, V. Lomakin, E. E. Fullerton, “Thermal stability of patterned Co/Pd nanodot arrays,” Applied Physics Letters 100 (10), 102401 (2012). The dissertation author was the contributing author to this article.
11.4 Bit Patterned Media with Vertical and Lateral Exchange: Design Considerations for 4 Tb/in$^2$ and 10 Tb/in$^2$ Recording

The reliability with which bits are written and stored on BPM depends closely on the width of the switching field distribution (SFD), as explained in section 11.2. The SFD is a measure of the spread in the amplitudes of the switching fields of the patterned islands comprising the media. The narrower the SFD, the more dependable is the recording. The broader the SFD, the greater is the bit-error frequency. As mentioned earlier, the SFD is in part due to variations in intrinsic properties of the media, such as easy axis orientation and saturation magnetization, and partly due to variations in extrinsic properties, such as island shape, position, and dipolar interactions. The dipolar contribution to SFD broadening was shown in many cases to be comparable to or even dominate over other contributions. Dipolar interactions have also been shown to compromise thermal stability of recorded bits. The extent to which dipolar interactions affect switching field distributions and thermal stability, and subsequently system performance, depends closely on the areal density, materials properties, and the architecture of the media, as well as the recording scheme and field profiles. The remainder of this section presents an assessment of the potential of heterogeneous capped bit patterned media and other proposed patterned media designs (Fig. 11.17) for ultra-high density magnetic recording with respect to writability, switching field distributions, and thermal stability at areal densities of 4 and 10 Tb/in$^2$.

11.4.1 Introduction to Capped Bit Patterned Media

Capped BPM (CBPM), which is comprised of magnetically hard patterned islands coupled to a continuous low anisotropy film, was recently introduced to address the challenge of dipolar broadening of SFDs [Ouchi and Honda, 2010] (Fig. 11.17d). In this design, the continuous capping layer enables compensation of dipolar interactions through lateral exchange between the bits, which is tuned to counterbalance the effects of the magnetostatic fields and reduce SFDs. These media can also reduce the switching fields. However, due to optimization towards a minimum SFD, the potential of the capping layer in explicitly reducing switching fields may not be fully exploited [Shiroishi et al., 2009]. Moreover, the domain walls in the capping layer can reduce media stability for
In this work we investigate the potential of heterogeneous CBPM (and other recently proposed BPM designs) for ultra-high density magnetic recording in terms of writability, SFDs, and thermal stability. Mechanisms leading to reduced switching fields and SFDs in different BPM designs are described. Effects of the capping layer on media stability and its optimization are examined. To achieve a maximum reduction in switching fields at minimal SFDs, ECC (exchange coupled composite) elements can be used in concert with the continuous capping layer (Fig. 11.17e). The capping layer may be coupled ferromagnetically or antiferromagnetically to the patterned bits. We show that in such media a simultaneous optimization for reduced SFDs and improved thermal stability is possible. In the AFC-composite-CBPM (AFC-CCBPM) design, the capping layer may also be optimized to suppress magnetostatic interference effects in the readback response (section 11.5).

11.4.2 Writability and Switching Field Distributions

Magnetostatically Induced Switching Field Distributions

Though media performance depends on a number of factors, such as the head design (e.g., integration with energy delivery mechanisms such as HAMR or MAMR)
and writing scheme (e.g., shingled writing [Kasiraj and Williams, 2005]), we will focus on switching fields and SFDs obtained assuming conventional recording systems. The procedure used here will allow for generalized conclusions, which can be extended to a more elaborate description of the recording system and process.

Presuming a uniform two-dimensional array of identical magnetic islands, the width of the SFD is due to dipolar interactions exclusively, and can be evaluated as the difference in switching fields between a bit surrounded by bits of the same magnetization direction (parallel configuration, Fig. 11.18a) and oppositely magnetized bits (antiparallel configuration, Fig. 11.18b). Generally, the dipolar contribution of the first and second nearest-neighbor bits accounts for most of the spread in switching fields. Hence, the third nearest neighbors can typically be omitted from the calculation of magnetostatically induced SFDs. A model consisting of only several nearest array elements surrounding the element to be switched is used. In Figs. 11.21–11.24 and Fig. 11.27, an array of only 3 elements is considered, as it is sufficient for studying the behavior and trends. For more complete media characterization in Figs. 11.19 and 11.25, a five-by-five square array of bits is used to quantify the magnetostatically induced SFDs. Square and staggered arrays lead to very similar results when the inter-island spacing is comparable to the island dimensions.

One solution to limit the extent of dipolar interactions in regular homogeneous or ECC BPM is to lower the saturation magnetization of the magnetic layer(s). Though this would result in a narrower SFD, it would also increase the anisotropy field, thus leading to a higher switching field and an associated writability problem. To demonstrate the tradeoff between writability and SFDs, we have carried out simulations on homogeneous and CBPM at 4 Tb/in$^2$, considering a five-by-five element array. The simulations were performed using a finite differences micromagnetic solver [Lomakin et al., 2007], and verified using *femme*, a finite element package [Suess et al., 2002, Dittrich et al., 2002, Scholz et al., 2003], which was also used for the energy barrier calculations in section 11.4.3. The results were obtained by integrating the Landau-Lifshitz Gilbert equation in time, with all fields accurately accounted for (exchange, anisotropy, magnetostatics, Zeeman). In both the homogeneous and CBPM model the net thickness of the patterned elements was chosen to be 15 nm (larger thickness would imply increased requirements on the write-field gradient [Schabes, 2008]), the anisotropy of the hard element ($H_K = 5$ kOe) was chosen to comply with $K_uV/k_B T = 55$ (for $T = 300$ K), and the applied field was directed
Figure 11.19: Plot indicating that the tradeoff between switching fields and SFDs that affects homogeneous BPM can be resolved by the capped BPM structure. The solid and dashed lines indicate the switching field of the central bit in the parallel (Fig. 11.18a) and antiparallel (Fig. 11.18b) configuration, respectively, for (black) homogeneous BPM and (red) capped BPM. Structural and material parameters for homogeneous and CBPM are given in Table 11.2 for 4 Tb/in$^2$.

vertically (see caption for details). Figure 11.19 shows the switching fields for homogeneous (black curve) and capped BPM (red curve) versus the saturation magnetization of the hard layer. The solid and dashed lines correspond to the switching fields, $H_{\text{P}}^{\text{sw}}$ and $H_{\text{AP}}^{\text{sw}}$, of the central bit obtained for the parallel (Fig. 11.18a) and antiparallel case (Fig. 11.18b), respectively. The discrepancy between the two field values represents the SFD. For homogeneous BPM, the SFD is large for large $M_s$ (corresponding to low switching fields for a fixed thermal barrier). For example, for $M_s = 950$ emu/cm$^3$ and magnetocrystalline anisotropy energy density $K_u = 2.38$ Merg/cm$^3$ (corresponding to an anisotropy field $H_K = 5$ kOe), the SFD for the homogeneous BPM is 70% of the mean switching field. Such a large SFD would pose major restrictions on the write field gradients, synchronization accuracy, and media patterning fidelity [Schabes, 2008]. To relax these restrictions, the ratio of the dipolar field to the switching field would have to be substantially reduced, either by increasing media anisotropy or reducing saturation magnetization. However, this would worsen the writability problem and could compromise
the readback signal intensity. The advantage of the CBPM design, as seen in Fig. 11.19, is that it is able to significantly reduce the SFD, thus allowing reliable recording at low switching fields. Here, the CBPM structure has been optimized towards minimal SFD at a hard layer saturation magnetization of 950 emu/cm$^3$. The tunability of the material parameters of the capping layer allows optimization towards minimal SFDs for arbitrary hard layer material parameters.

We now describe details of the lateral and vertical exchange interactions in CBPM, and analyze the dependence of the switching field and SFD on materials parameters of the capping layer. A single-track capped BPM model consisting of three islands is sufficient to illustrate the main principles and provide understanding of the optimization process. Figures 11.20a and 11.20b illustrate the magnetization configurations of a track of capped BPM when the central island is oriented parallel and antiparallel to its neighbor-islands. The structure is characterized by vertical exchange across the island-cap interface, and lateral exchange across the length of the capping layer. The degree of exchange coupling between adjacent islands can be modulated by tuning the strength of lateral and vertical exchange. Vertical exchange is modulated through the interfacial coupling strength (or energy density), $J_{int}$, which in practice can be tuned by varying the composition and thickness of a thin spacer layer deposited between the capping layer and the patterned
Figure 11.21: Switching fields versus saturation magnetization of the capping layer in CBPM for the central bit in the parallel (solid lines) and antiparallel (dashed lines) configurations for capping layer thicknesses, $t_{\text{cap}} = 1$ nm (black lines), $t_{\text{cap}} = 3$ nm (blue lines), and $t_{\text{cap}} = 6$ nm (green lines). Remaining parameters are the same as in Table 11.2 for 4 Tb/in$^2$, with the exception of $M^s_h = 950$ emu/cm$^3$ and interfacial coupling energy density $J_{h/\text{cap}} = 1$ erg/cm$^2$.

hard layer [Parkin et al., 1990]. The strength of the lateral exchange depends on the exchange length of the capping layer, $l_{\text{cap}}^\text{ex} \approx \sqrt{A_{\text{ex}}^\text{cap}/M^s_{\text{cap}}}$, where $A_{\text{ex}}^\text{cap}$ is the exchange constant, and $M^s_{\text{cap}}$ is the saturation magnetization. A large $l_{\text{ex}}^\text{cap}$ implies increased stiffness in the capping layer, hence stronger lateral exchange coupling. Because the capping layer stiffness favors uniform magnetization (Fig. 11.20a), the exchange interaction opposes the dipolar interaction (Fig. 11.20b). The magnetocrystalline anisotropy of the capping layer also has an influence on the extent to which magnetostatic interactions are compensated during island reversal, and has important implications for the media stability.

Figure 11.21 illustrates the dependence of the switching fields for the parallel configuration ($H^P_{\text{sw}}$, solid line) and antiparallel configuration ($H^{\text{AP}}_{\text{sw}}$, dashed line) on the saturation magnetization $M^s_{\text{cap}}$, for capping layer thickness $t_{\text{cap}} = 1$ nm, 3 nm and 6 nm. When $M^s_{\text{cap}}$ is large, the exchange coupling between the bits is weak, and the dipolar interaction dominates, resulting in $H^P_{\text{sw}} < H^{\text{AP}}_{\text{sw}}$. As $M^s_{\text{cap}}$ is reduced, the exchange interaction becomes dominant, and $H^P_{\text{sw}} > H^{\text{AP}}_{\text{sw}}$. The point of intersection between the solid and dashed lines ($H^P_{\text{sw}} = H^{\text{AP}}_{\text{sw}}$) indicates that the effect of dipolar interactions on
Table 11.2: Structural and material parameters used to model different BPM designs.

In all models the exchange constant was $A_{\text{ex}} = 1.0 \times 10^{-6}$ erg/cm and the high-damping regime was assumed.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>HBPM</th>
<th>CBPM</th>
<th>HBPM</th>
<th>CBPM</th>
<th>ECC</th>
<th>Ledge</th>
<th>FC-CCBPM</th>
<th>AFC-CCBPM</th>
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<td>500-900</td>
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<tr>
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<td>20</td>
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<td>0.75</td>
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</table>

the switching fields has been fully compensated by the exchange interaction.

Figure 11.22 shows the dependence of $H_{\text{sw}}^P$ and $H_{\text{sw}}^{\text{AP}}$ on the interfacial coupling strength, $J_{h/cap}$, for three values of capping layer anisotropy, $K_{\text{cap}}^u = 0, 1, \text{and} 2$ Merg/cm$^3$. As $J_{h/cap}$ increases, so does the inter-island exchange coupling, and hence for large $J_{h/cap}$ we have $H_{\text{sw}}^P > H_{\text{sw}}^{\text{AP}}$. Furthermore, the greater the $K_{\text{cap}}^u$, the greater the effect of the exchange interaction on switching fields. This is because in the antiparallel configuration the magnetization of the capping layer is not in perfect alignment with the easy axis, and, under a reduced applied field, can cross over to the opposite preferential direction, thereafter assisting the applied field in reversing the hard island through an increased exchange field.

Another parameter which may serve to tune the exchange interaction is the exchange constant $A_{\text{ex}}^\text{cap}$. It may be preferable to have a relatively small $A_{\text{ex}}^\text{cap}$ to prevent the exchange interaction from being too strong. The exchange constant can be varied by tuning the Curie temperature through compositional adjustment [Albrecht and Schabes, 2009] or by ion-irradiation [Chappert et al., 1998, Stanescu et al., 2008]. Irradiating only parts of the capping layer between patterned islands would reduce lateral exchange while preserving vertical exchange, thus enabling significant reduction in both switching fields.
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Figure 11.22: Switching fields versus interfacial coupling between capping layer and hard island for central bit in the parallel (solid lines) and antiparallel (dashed lines) configurations for capping layer anisotropy, $K_u^{cap} = 0$ Merg/cm$^3$ (black lines), $K_u^{cap} = 1$ Merg/cm$^3$ (blue lines), and $K_u^{cap} = 2$ Merg/cm$^3$ (red lines). The simulation parameters (apart from those indicated in the figure above), are the same as the ones listed in Table 11.2 for 4 Tb/in$^2$, except for $M_r^{cap} = 1050$ emu/cm$^3$.

Reduced lateral exchange would enable large thicknesses of the capping layer. As a result, the capping layer can further be replaced by the soft magnetic underlayer (SUL), thus allowing reducing switching fields, SFDs, controlling the head field and readback, and potentially simplifying the fabrication process. Another possible means to tune lateral exchange is to use a soft granular capping layer (with grains smaller than the BPM elements) and modulate the inter-granular exchange coupling [Qin and Zuo, 2010].

To achieve a maximal reduction in both switching fields and SFDs, assuming lateral exchange has not been previously reduced, we introduced a new design, referred to as capped-composite-BPM (CCBPM), in which ECC elements are coupled to the capping layer, instead of homogeneous elements (Fig. 11.17c). Because the ECC elements ensure low switching fields [Suess et al., 2005, Victora and Shen, 2005a, Fullerton et al., 1999], the capping layer may be coupled to the hard layer either ferromagnetically or antiferromagnetically. Figure 11.23 illustrates that the switching fields for FC and AFC-CCBPM are considerably lower than for CBPM, while the SFD is equally reduced. Conversely, ECC and ledge BPM are shown to have very wide SFDs, represented by the
Figure 11.23: Comparison of switching fields and SFDs at 10 Tb/in$^2$ for (a) homogeneous BPM (gray), CBPM (blue), and for (b) ECC BPM (magenta), ledge BPM (cyan), FC-composite-capped BPM (black), and AFC-composite-capped BPM (red). Solid and dashed lines correspond to the switching field of central bit in the parallel (Fig. 11.20a) and antiparallel (Fig. 11.20b) configuration, respectively. The discrepancy between a solid and dashed curve (of the same color) indicates the width of the SFD of the corresponding capped structure. Switching fields for the capped designs are shown at different values of capping layer saturation magnetization, $M_{\text{cap}}^s$ (horizontal axis). The span of the SFD for BPM designs not consisting of a capping layer is color-shaded for ease of comparison. The range of $M_{\text{cap}}^s$ in each plot was chosen to capture the balance point in capped designs, where the solid and dashed lines intercept and the SFD is at a minimum. The location of the balance point relative to the $M_{\text{cap}}^s$ depends on the intensity of dipolar and exchange interactions, which are different for the capped structures in the left and right plot. Corresponding values of structural and material parameters for the different layers in each design are listed in Table 11.2 for 10 Tb/in$^2$.

Materials Contribution to Switching Field Distributions

Before moving on to a discussion of thermal stability in the next section, it is useful to inspect the materials contribution to SFD in capped BPM structures. Preceding figures relating the dependence of switching fields on $J_{\text{int}}$, $M_{\text{cap}}^s K_u^{\text{cap}}$, and $t_{\text{cap}}$ already gave some insight to the SFD caused by structural and materials fluctuations in the capping

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corresponding shading in Fig. 11.23b.

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layer. What follows is an investigation of the SFDs caused by materials fluctuations occurring in the hard layer. Figure 11.24 illustrates the sensitivity of the switching fields for homogeneous BPM, capped BPM, ECC BPM, and AFC-CCBPM on hard layer anisotropy energy density. When interfacial coupling is low, CBPM responds to fluctuations in hard layer material properties similarly as homogeneous BPM (Fig. 11.24a). If the interfacial exchange between a soft and a hard layer is increased, the switching field dependence on hard layer anisotropy is significantly altered due to a change in reversal mode, as seen in Fig. 11.24b for ECC as well as FC and AFC-CCBPM [Victora and Shen, 2005a]. The CCBPM designs allow significant reduction in both dipolar and material induced SFDs. A further reduction in intrinsic SFDs can be achieved using multilayer materials with uncorrelated distributions of material properties [Krone et al., 2010].

11.4.3 Thermal Stability

In order to ensure high thermal stability of recorded data, the energy barrier $E_b$, separating the up and down magnetization directions, is required to be at least $45k_BT$, where $k_B$ is the Boltzmann constant and $T = 300$ K [Weller and Moser, 1999]. In
BPM with uncoupled elements dipolar interactions can significantly reduce the thermal stability of the media, because the stray magnetostatic fields emanating from the bits act as an effective applied field, $H_a^{\text{eff}}$, reducing the energy barrier between the two stable states by around $KV[1 - (1 - H_a^{\text{eff}}/H_0)^\alpha]$, where $H_0$ is the short-time coercivity of the island, and $\alpha$ specifies the angle dependence to the effective applied field [Sharrock and McKinney, 1981]. Below we investigate thermal stability of several media types and show that CBPM can lead to increased energy barriers. The energy barriers for all results were computed with **femme** [Suess et al., 2002, Scholz et al., 2003] using the nudge elastic band method [Dittrich et al., 2002].

Figure 11.25 illustrates the thermal reversal of a central island in a five-by-five array of homogeneous bits at 4 Tb/in$^2$, with thermal stability ratio $KuV/k_BT = 55$, and anisotropy field $H_K = 5$ kOe. The energy barrier corresponding to the transition from the parallel to the antiparallel configuration, $T^{P\rightarrow AP}$, is much smaller than the energy barrier for the reverse transition, $T^{P\leftarrow AP}$, and the energy path is asymmetric around the saddle point (Fig. 9a). This asymmetry is caused by the change in polarity of the dipolar field acting on the central island in the parallel and antiparallel configuration. As a result, the energy barrier associated with $T^{P\rightarrow AP}$ is four times smaller than that of $T^{P\leftarrow AP}$, and well below the acceptable limit of $45 k_BT$. A way to recover stability in homogeneous BPM would be to increase $H_K$ of the media, which would lead to higher switching fields.

CBPM provides an alternative means to regain media stability that does not rely on increasing media anisotropy. Figure 11.25b illustrates the minimum energy path for thermal reversal of the central bit in a five-by-five array of capped bits, with hard layer material and structural parameters identical to those of homogeneous BPM (see caption of Fig. 11.25 for details). Apart from the improvement in symmetry about the saddle point, the energy barrier for both the $T^{P\rightarrow AP}$ and $T^{P\leftarrow AP}$ transitions in capped BPM is well above $45 k_BT$, in contrast to homogeneous BPM. The energy barrier corresponding to the $T^{P\rightarrow AP}$ transition is improved in capped BPM because this transition necessitates the formation of domain walls in the capping layer (as in Fig. 11.20b). To achieve a $T^{P\rightarrow AP}$ transition, an added exchange energy required to obtain the domain wall needs to be supplied. For the reverse transition $T^{P\leftarrow AP}$, the energy barrier which was in homogeneous BPM inflated by the dipolar interaction, in capped BPM is lowered by the energy provided to the system through the expulsion of the domain walls in the capping
Figure 11.25: Minimum energy path (MEP) between the parallel (Fig. 11.18a) and antiparallel (Fig. 11.18b) configuration for (a) homogeneous BPM and (b) capped BPM. For homogeneous BPM the energy barriers for the forward and reverse transition are markedly different due to uncompensated dipolar interactions. In CBPM, the stability is improved. Structural and material parameters are listed in Table 11.2 for 4 Tb/in\(^2\).

Because the modes for field-assisted and thermal reversal differ [Suess, 2007], it is not obvious whether capped BPM can resolve the SFD problem and retrieve media stability simultaneously. However, both the simulations leading to the SFD results of Fig. 11.19 and the stability calculations presented in Fig. 11.25b involved the same capped BPM model, with identical structural and material parameters, demonstrating that a simultaneous optimization toward minimal SFDs and improved thermal stability is indeed possible.

Reducing SFDs in CBPM, however, does not necessarily imply an improvement in stability. A set of parameter values leading to minimal SFDs may in fact result in stability reduction. Understanding the details of exchange interactions in laterally and vertically coupled systems is therefore essential to overall media optimization. In the following, we investigate the influence of the capping layer on the thermal stability of capped structures, study the dependence of the energy barriers on materials parameters of the capping layer, and explore means to maximize stability.

In order to study thermal stability it is useful to look at the equilibrium states of capped BPM for different media parameters and recorded configurations [Goll and Macke, 2008]. Figure 11.26a shows the expected equilibrium magnetization configuration...
Figure 11.26: Possible equilibrium states for capped BPM. Equilibrium configuration and stability depend both on the geometry and material properties of the patterned islands and the capping layer, as well as the strength of exchange coupling at the interface.

when all bits are equally oriented (parallel configuration) and the interfacial coupling, $J_{h/cap}$, between the hard layer and capping layer is strong, and/or when the capping layer has a moderate anisotropy, $K_{u/cap}$. If $J_{h/cap}$ and $K_{u/cap}$ are relatively low, and the saturation magnetization of the capping layer, $M_{cap}s$, is high, the magnetization in the capping layer has a tendency to lie in plane due to magnetostatic interactions (Fig. 11.26b). Figures 11.26c-f illustrate the equilibrium magnetization states that occur for the antiparallel configuration under different media parameters. For the larger part of the CBPM parameter space, the magnetization configuration in Fig. 10c is prevalent. That is, the magnetization in the capping layer for a state of alternating bits tends to be largely in-plane due to exchange-stiffness [Moser et al., 2003]. A more symmetric magnetization distribution results (Fig. 11.26c) when the capping layer is thin, and $J_{h/cap}$ and/or $K_{u/cap}$ is increased, or when the exchange constant, $A_{ex/cap}$, is reduced (by irradiation, for example [Chappert et al., 1998]). The domain wall formed between the oppositely oriented bits in single-track CBPM is usually a Néel wall due to dipolar interactions and a relatively large exchange length. However, if $M_{cap}s$ is significantly reduced, while a small exchange length is maintained through $A_{ex/cap}$, a Bloch wall is possible (Fig. 11.26d).
Finally, if the capping layer is sufficiently stiff magnetically, and/or has too large an anisotropy, the exchange field on the capping layer from the island above may be too weak to influence its magnetization in the same direction, resulting in an adverse stable state depicted in Fig. 11.26f.

With these possible equilibrium states in mind, we consider the dependence of the energy barriers separating the parallel and antiparallel configurations on the material parameters of the capping layer. The inset in Fig. 11.27 shows the transition from the parallel to the antiparallel configuration, \( T_{\text{thermal}}^{P \rightarrow AP} \), indicated by the blue arrow, and the reverse transition \( T_{\text{thermal}}^{P \leftarrow AP} \), indicated by the red arrow. The blue and red lines in the plot of Fig. 11.27 show the dependence of the energy barriers associated with these transitions, \( E_{h}^{P \rightarrow AP} \) and \( E_{b}^{P \leftarrow AP} \), on the uniaxial anisotropy, \( K_{u}^{\text{cap}} \), of the capping layer. The thermal stability for the parallel configuration, \( E_{h}^{P \rightarrow AP} \), is seen to grow with \( K_{u}^{\text{cap}} \) on the interval from \( K_{u}^{\text{cap}} = 0 \) to approximately \( K_{u}^{\text{cap}} = 3.5 \) Merg/cm\(^3\), and saturating thereafter. This behavior is expected, because, for the parallel configuration, an increase in capping layer anisotropy adds to the net anisotropy of the system, thus the stability initially increases. Once the capping layer anisotropy field exceeds the exchange field provided by the coupling between the island and the capping layer, the energy barrier, \( E_{b}^{P \rightarrow AP} \), grows no longer with \( K_{u}^{\text{cap}} \). In other words, the energy required to independently reverse the magnetization in the portion of the capping layer beneath the island becomes greater than the energy of the interfacial domain wall created thereof. Indeed, when the anisotropy field exceeds the exchange field, the state in Fig. 11.26f becomes a possible equilibrium state for the antiparallel configuration, which further explains the behavior of \( E_{b}^{P \leftarrow AP} \) with \( K_{u}^{\text{cap}} \) (red line). Greatest thermal stability is therefore obtained when \( K_{u}^{\text{cap}} \) is relatively small.

Another way to avoid the equilibrium configuration of Fig. 11.26f is to increase the coupling strength, \( J_{h/cap} \), between the capping layer and the hard islands. Though this would prevent the state of Fig. 11.26f from occurring, the energy barrier for the \( T_{\text{thermal}}^{P \leftarrow AP} \) transition would generally suffer. A large \( J_{h/cap} \) implies the existence of condensed high-energy domain walls in the antiparallel configuration. During thermal reversal the energy provided by the domain walls as they unfold exceeds the dipolar contribution, and lowers the net energy of the system. Furthermore, as seen in Fig. 10c, the exchange field exerted by the capping layer on the central element at equilibrium causes the moment in the hard island to noticeably deviate from the easy axis. Hence, the anisotropy energy
Figure 11.27: Energy barriers for the transition from the parallel to the antiparallel configuration and vice versa, versus capping layer anisotropy, for $M_{\text{cap}} = 1050 \text{ emu/cm}^3$ and $J_{h/\text{cap}} = 0.33 \text{ erg/cm}^2$. Remaining parameters, apart from $K_{\text{cap}}^u$ which is here a variable, are the same as in Table 11.2 for CBPM for 10 Tbit/in$^2$.

of the island in its initial equilibrium state is reduced in comparison to the full island anisotropy, and the absolute energy barrier for the $T_{\text{thermal}}^{P \rightarrow AP}$ transition is reduced. Overall, increasing $J_{h/\text{cap}}$ from 1 erg/cm$^2$ to 4 erg/cm$^2$ results in a two-fold reduction in media stability, for the chosen parameters.

The thermal stability can also be tuned through the saturation magnetization, $M_{\text{cap}}^s$, and exchange constant, $A_{\text{ex}}^{\text{cap}}$, of the capping layer. Presuming a relatively small $J_{h/\text{cap}}$ and $K_{u/\text{cap}}^c$, the energy barriers $E_{b/\text{cap}}^{P \rightarrow AP}$ and $E_{b/\text{cap}}^{P \rightarrow AP}$, will not be drastically effected by adjustments in $M_{\text{cap}}^s$ or $A_{\text{ex}}^{\text{cap}}$, providing a decent range over which both SFDs and thermal stability may be optimized. The behavior of $E_{b/\text{cap}}^{P \rightarrow AP}$ and $E_{b/\text{cap}}^{P \rightarrow AP}$ with $M_{\text{cap}}^s$ and $A_{\text{ex}}^{\text{cap}}$ is similar to that of $H_{\text{sw}}^{P}$ and $H_{\text{sw}}^{AP}$ within this range.

Thermal stability can also be improved by exploiting domain wall assisted switching. For example, ECC BPM allows much larger hard-layer anisotropies to be used for the same switching fields as in homogeneous BPM [Suess et al., 2005]. This improves media stability without compromising writability. However, ECC BPM can suffer from large SFDs (Fig. 11.23b) due to the increased magnetic volumes of the composite structures, which can also be a source of stability loss. The FC and AFC-CCBPM designs resolve
these issues, minimizing SFDs, while maximizing stability and writability on account of lateral and vertical coupling which can tuned.

11.4.4 Summary

Dipolar interactions play a significant role in the broadening of SFDs and in deterioration of thermal stability, which significantly limit the performance of magnetic recording on BPM at ultra-high areal densities. For a five-by-five array of homogeneous BPM at 4 Tb/in$^2$ and media anisotropy $H_K = 5$ kOe it was found that the SFD was 70% of the mean switching field, while the stability was reduced to less than 50% of the stability of a single magnetostatically isolated island, having the same material parameters. Use of ECC elements can improve stability for the same switching fields, but does not help with narrowing SFDs. We have shown that CBPM and its extensions can address simultaneously the problem of SFDs and stability loss, leading to significant improvements by offsetting dipolar effects through exchange interactions introduced through the coupling with a continuous capping layer. At larger areal density and media anisotropy, the CCBPM designs (CBPM with ECC elements) demonstrated improved writability over homogeneous and capped BPM, and significantly narrower SFDs in comparison to ECC and ledge BPM. The switching field and energy barrier dependence on capping layer material properties were discussed. The rich range of tuning parameters offered by the capped designs allows optimization leading to minimal SFDs, improved stability, and greater writability, which can be achieved for arbitrary areal density and media geometry. With these characteristics, CBPM presents itself as a promising candidate for ultra-high density magnetic recording applications.

Acknowledgements: Section 11.4 in Chapter 11 is a reprint of the journal article: M. V. Lubarda, S. Li, B. Livshitz, E. E. Fullerton, V. Lomakin, “Reversal in bit patterned media with vertical and lateral exchange,” IEEE Transactions on Magnetics 47 (1), 18–25 (2011). The dissertation author was the primary author to this article.
11.5 Antiferromagnetically Coupled Capped Bit Patterned Media: Design Considerations for 6 Tb/in$^2$ Recording

This section focuses on micromagnetic modeling of a bit patterned media where a two-dimensional array of patterned composite islands is antiferromagnetically coupled to a continuous capping layer. This media allows optimization of writability, switching field distributions, and readback response. Lateral and vertical exchange compensates the dipolar interaction between islands while antiferromagnetic coupling modulates the high-density readback response.

11.5.1 Motivation

While BPM is envisioned to extend the accessible areal densities of magnetic storage, it will face similar challenges as perpendicular magnetic recording (PMR) as device geometry is reduced to yet smaller dimensions. The problem of writability reemerges at very high areal densities, where, in order to compensate for reduced bit sizes and maintain thermal stability, the anisotropy must be increased to such values that the switching fields may no longer be within the range of conventional write heads. Furthermore, high proximity of patterned bits implies strong magnetostatic interactions resulting in significant dipolar broadening of switching field distributions (SFDs), which, together with the materials and microstructural contributions to intrinsic SFDs, may lead to unreliable operation. The capacity to resolve the magnetization of the recorded bits also diminishes, as interbit spacing shrinks, and magnetostatic interference from neighboring bits increases. The combined writability requirements, increased SFDs, and a compromised readback are major challenges for achieving ultra-high areal densities [Chunsheng et al., 2006, Richter, 2007, Lomakin et al., 2007, Hellwig et al., 2007].

11.5.2 Design Details and Modeling

To address these challenges we present the antiferromagnetically-coupled composite-capped BPM (AFC-CCBPM) design characterized by improved writability, reduced SFDs, and modulated readback response. The design consists of a two-dimensional array of patterned exchange-coupled composite (ECC) elements [Suess et al., 2005, Victora and Shen, 2005a, Fullerton et al., 1999] antiferromagnetically coupled to a continuous lower-anisotropy film (referred to as the capping layer), as shown schematically in Fig. 11.28a.
Figure 11.28: (a) Illustration of the proposed AFC-CCBPM design showing a five-by-five array of ECC elements antiferromagnetically coupled to a continuous capping layer. To the right, the remanent spin configurations are shown for (b) uniform and (c) alternating magnetization states.

All layers possess perpendicular uniaxial anisotropy. ECC elements are employed because they can be optimized for high writability with limited or no cost to thermal stability [Suess et al., 2005, Suess, 2007] and reduced sensitivity to distributions in the anisotropy energy density and easy-axis direction [Victora and Shen, 2005a, Victora and Shen, 2005a]. Graded multilayer elements could be used as well to further boost the reduction in switching fields [Goncharov et al., 2007]. The role of the capping layer is to introduce lateral ferromagnetic exchange coupling between the elements of the BPM media that compensates the magnetostatic coupling [Li et al., 2009a, Albrecht and Schabes, 2009]. The role of the antiferromagnetic coupling is to further allow the capping layer to improve the readback response. We show that the recording and readback performance of the proposed media has distinct advantages over the performance of a number of recently reported BPM designs.

To investigate the writability, SFD, and readback response of AFC-CCBPM, we employ micromagnetic simulations based on the Landau-Lifshitz-Gilbert equation, taking into account all energy terms via the effective field, and ensuring good convergence through proper discretization [Lomakin et al., 2007]. The simulated structure is a five-by-five array of identical, equally spaced ECC elements antiferromagnetically coupled to a continuous capping layer (Fig. 11.28). A five-by-five array was found sufficient for the study; the dipolar contribution of the third nearest-neighbor-bits on the SFD was found to be insignificant. The areal density of the media is 6 Tb/in².
Material and structural parameters of the optimized structures are given in Table 11.3. In all the simulations the recording field is applied uniformly parallel to the easy axis over a region of space defined by the central ECC element and the fraction of capping layer beneath it. The dependence of the switching field on the magnetization states of surrounding bits is determined in order to characterize SFDs arising from dipolar interactions. The particular applied field profile is chosen to demonstrate how the media performance can be optimized. The performance can also be optimized for a wide range of other more realistic head-field profiles.

**Table 11.3:** Summary of simulation parameters used for each design (layer thickness \( t \), element width \( w \), interbit spacing \( \Delta b \), saturation magnetization \( M_s \), anisotropy field \( H_K \), and interfacial coupling \( J \)). The indices \( h \), \( s \), and \( \text{cap} \) correspond to the hard, soft, and capping layer, respectively. The media density, net thickness of islands, and hard-layer thermal stability ratio are, respectively, \( AD=6 \text{ Tb/in}^2 \), \( t=10 \text{ Tb/in}^2 \), and \( K_u V/ k_B T = 60 \) \( (T = 400 \text{ K}) \) for all designs in the table. The exchange coupling constant is \( A_{\text{ex}} = 1.3 \times 10^6 \text{ erg/cm} \) for all layers. The high damping regime is assumed in all simulations.

<table>
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<th>HBPM</th>
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<th>AFC ECC</th>
<th>CBPM</th>
<th>FC-CCBPM</th>
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11.5.3 Configurational Dependence on Switching Fields and Switching Field Distributions

We start with showing the tradeoffs in conventional BPM designs for a given areal density. The thickness of the BPM islands in all designs is $t = 10$ nm. Figure 11.29 shows the switching fields and SFDs for several BPM designs. For the conventional (laterally uncoupled) designs the dipolar SFDs are defined as the difference between the fields of parallel and anti-parallel configurations. In the former configuration the initial states of all the bits are up and the central bit is to be switched down, whereas in the latter configuration the central bit is down and is to be switched up. We note that SFDs related to other states can be smaller. When considering recording performance there are distinct probabilities for the system to be in a particular state. This may result in the effective magnetostatically-induced SFDs being less severe than calculated here but still important to system performance.

From Fig. 11.29, the first five designs are characterized by a tradeoff between writability and SFDs. Homogeneous BPM has a large mean switching field $\langle H_{sw} \rangle$ and a relatively low SFD (Fig. 11.29). Reducing $\langle H_{sw} \rangle$ in homogeneous BPM while maintaining...
Figure 11.30: Switching fields of the central bit for different magnetization patterns of surrounding bits versus capping layer anisotropy for AFC-CCBPM. The range spanned by the data indicates the width of the SFD at any given anisotropy value (see Table 11.3 for parameter values).

A fixed media stability implies increasing $M_s$, which enhances the dipolar coupling between islands and broadens the SFD. In composite BPM, the switching field is reduced based on the exchange-spring mechanism, but the resulting reduction in $\langle H_{sw} \rangle$ leads to an increase in the SFD. Furthermore, if the soft section has a large $M_s$ to maximize reduction in $\langle H_{sw} \rangle$, the dipolar coupling and resulting SFD is increased (Fig. 11.29). AFC-composite-BPM, on the other hand, has lower SFDs, but high switching fields [Piramanayagam et al., 2009, Ranjbar et al., 2010]. The tradeoff between the two quantities is partially resolved for the case of capped BPM [Li et al., 2009a]. From these results it is evident that the conventional BPM designs lead to a tradeoff between the switching field and SFD. It is also evident that SFDs due to dipolar broadening can reach significant values at ultra-high densities.

The situation is very different for the (FC and AFC) CCBPM designs, which significantly and simultaneously reduce both switching fields and SFDs. For these designs the SFDs are defined as the difference between the maximal and minimal switching fields over all possible initial configurations (in the case of laterally uncoupled BPM, only the parallel and antiparallel configurations needed to be considered). Figure 11.30 shows the
switching fields of the central bit for eight patterns of magnetization states (illustrated to the right) plotted against different values of cap anisotropy (we verified that the maximal and minimal states can be found from these eight configurations). For $K_u^{\text{cap}} = 3.5 \times 10^6$ erg/cm$^3$, the maximum SFD is just under 10% of the mean switching field of 7.5 kOe, well below the anisotropy field of the hard layer $H_K = 35$ kOe. With these simultaneous improvements in writability and SFDs, the CCBPM model shows distinct advantages over all other presented designs. The dependence on $K_u^{\text{cap}}$ shown in Fig. 11.30 shows the possibility to optimize the media by modulating $K_u^{\text{cap}}$. Other parameters can be used in optimization to achieve similar or better performance. The media can also be optimized for a specified recording field profile, hard-layer parameters, and areal density. The importance of each parameter in the optimization process will be addressed below.

### 11.5.4 Optimization Considerations

The values of all material parameters used in the modeling and listed in Table 11.3 are consistent with known materials. The magnetization values and anisotropy fields are below those of ordered FePt. Therefore, these values can be fulfilled by using (Fe, Co, Pt) alloys or multilayers. The AF coupling constants are typical of those corresponding to Ir, Rh and Ru interlayers, and the FM coupling constants are typical of those corresponding to Pd or Pt interlayers.

The improved performance of CCBPM, seen in Fig. 11.29, is attributed to domain-wall processes occurring in the media during reversal. In the case of AFC-CCBPM the soft ECC section begins to reorient, thus applying an exchange field to the hard element and significantly lowering the switching field. The magnetization in the capping layer tends to orient with the applied field and can oppose reversal (due to the AF coupling). However, the extent to which the capping layer moments align with the applied field depends on the direction and intensity of the exchange field resulting from inter-island coupling. Because the exchange interaction favors magnetization uniformity, lateral coupling assists alignment of the cap moments with the external field in the case of oriented bits (Fig. 11.28b), and opposes alignment in the antiparallel case (Fig. 11.28c). Since dipolar interactions favor nonuniform magnetization, the lateral and vertical exchange can be tuned to minimize dipolar broadening of SFDs. Another contribution to SFDs comes from material fluctuations and structural nonuniformity, which can be introduced during the material growth and patterning process. The use of ECC elements in the CCBPM
design reduces the switching field dependence on hard layer anisotropy [Victora and Shen, 2005a, Suess et al., 2005]. Further reduction of the influence of local distributions and grain structure on SFDs can be achieved by using uncorrelated multilayers [Krone et al., 2010]. Edge roughness is not expected to significantly affect the reversal mode since the island size does not exceed the exchange or domain wall length. Planar BPM obtained through ion-irradiation may further limit defects [Chappert et al., 1998], and can be designed to provide controlled lateral exchange.

Effective optimization of AFC-CCBPM and other capped BPM models requires understanding of how the capping layer parameters affect lateral exchange. For example, if the exchange length $t_{\text{ex}}^\text{cap} \approx \sqrt{A_{\text{ex}}^\text{cap}} / M_s^\text{cap}$ is less than the inter-bit spacing, the magnetization in the cap will be very stiff. If the interfacial coupling $J_{b/\text{cap}}$ is large, this will lead to too strong inter-island coupling, and the dipolar contribution to SFDs will be overcompensated. The anisotropy field $H_K^{\text{cap}} = 2K_u^\text{cap} / M_s$ plays a role in controlling the extent to which the cap moments align along the applied field, as discussed above. The thickness $t_{\text{cap}}$ determines the allowed exchange field at the hard/cap layer interface, and is an important parameter in controlling the capping layer contribution to the readback signal.

11.5.5 Readback Response

While FC and AFC-composite-CBPM have a similar writing performance (Fig. 11.29), the AFC design has important advantages in terms of the reading performance. The reciprocity principle was used to calculate the readback response for the BPM designs outlined in Fig. 11.29. The read head was modeled as a finite width MR sensor and infinitely wide shields [Karakulak et al., 2008]. Head width was chosen to be $W = 15$ nm with a thickness of the MR sensor $t = 3$ nm, and a gap between sensor and shield $g = 15$ nm. The pattern of magnetization states used in the reciprocity calculation is pattern (vii) of Fig. 11.30a. Such a pattern has been selected to emphasize the magnetostatic interference (or screening) effects neighboring bits can have on the central element during readback when the dimensions of the head (e.g., due to technological limitations) do not ideally conform to the media geometry. Figure 11.31a shows the calculated readback signal obtained for AFC-CCBPM, FC-CCBPM, as well as ECC-BPM, as the head flies over the central track of pattern (vii) in Fig. 11.30a. The screening effects have a noticeable influence on the readback signal for ECC-BPM and FC-CCBPM due to the
fields emanating from the neighboring composite elements, and, in the latter case, from the cap magnetization as well. A more robust signal results from AFC-CCBPM, where interference effects are in part compensated by the AFC capping layer, leading to a more consistent waveform. This is most clearly seen in the three-dimensional plot of Fig. 11.31a,c.

It is worthwhile noting that the antiferromagnetic coupling in AFC-CCBPM does not necessarily imply that the moments in the capping layer are in antiparallel alignment with the moments in the patterned elements. The magnetic configuration of the capping layer depends on the specific pattern of magnetization states of patterned bits. The capping layer moments will point to a larger extent out-of-plane as the number of equally oriented bits in a particular region increases (Fig. 11.28b). In the case of a distribution of alternating states, where the screening effects are uncorrelated and cancel out, the magnetization of the capping layer will point largely in-plane [Moser et al., 2003], and not appreciably participate in the readback response (Fig. 11.28c).
Figure 11.31d shows the effect of the soft underlayer (SUL) on the readback signal for the three media designs. The influence of magnetostatic interference on the readback signal for ECC and FC-CCBPM is seen to be enhanced due to the SUL. However, the SUL does not have the same effect on the response of AFC-CCBPM, indicating that this effect may be moderated through a proper choice of capping layer thickness, saturation magnetization, and other materials parameters.

Acknowledgements: Section 11.5 in Chapter 11 is a reprint of the journal article: M. V. Lubarda, S. Li, B. Livshitz, E. E. Fullerton, V. Lomakin, “Antiferromagnetically coupled capped bit pattern media for high density recording,” Applied Physics Letters 98 (1), 012513 (2011). The dissertation author was the primary author to this article.
12 Spin Valves

The current chapter focuses on design considerations for several spin valve applications, and discusses paths for overcoming important challenges for further improvements in performance. An all-perpendicular dual free layer spin valve, envisioned for use in magnetic random access memory, is proposed and analyzed using micromagnetic simulations [Yulaev et al., 2011]. It is shown that the new design lowers the threshold for current-induced switching and leads to improved switching rates. The ability to tailor effective damping through modulation of the softer free layer only provides an additional means for reducing the tradeoffs limiting spin valve scalability.

12.1 Applications and Challenges

Ever since the discovery of the giant magnetoresistance (GMR) and tunneling magnetoresistance (TMR) effects, researchers have been looking at ways to use spin valves to improve existing technologies and implement novel devices. The key advantages of spin valve-based magnetic devices are nonvolatility, low power consumption, scalability, and radiation hardness. The following sections review existing and potential applications of spin valves, including magnetic field sensors, magnetic random access memory (MRAM), spin valve logic, and spin-torque nanooscillators (STNOs).

12.1.1 Magnetic Field Sensors

The first commercialized GMR-based spin valve product was the read head, which was introduced into the magnetic recording system in 1997 [Childress and Fontana, 2005]. The simplified model of the GMR read head consists of a magnetic multilayer stack with metallic leads connected to its edges that allow currents to flow laterally in the film plane, as illustrated in Fig. 12.1a. Of the different layers in the stack, the three that
Figure 12.1: (a) Example of multilayer stack in GMR read head with metallic leads connected to its edges (current-in-plane geometry). (b) Example of multilayer stack in TMR read head with metallic leads connected directly from top and bottom (current-perpendicular-to-plane geometry).

play the central role in device operation are the free layer, the reference layer, and the nonmagnetic metal spacer layer. The free layer is magnetically soft with a magnetization direction free to move in response to the stray magnetic field emanating from the storage medium over which the head flies. The magnetization of the reference layer, on the other hand, is permanently set in the direction of the magnetization of the exchange-biased pinned layer to which it is ferromagnetically coupled. The resistance of the spin valve device depends on the relative alignment of the free and the reference layers due to the spin-dependent scattering rates (Fig. 12.2) [Valet and Fert, 1993]. The voltage therefore is used as the output signal from which the recorded magnetization state in the recording medium is inferred.

In terms of materials considerations, the free layer has to be both soft and provide a large GMR response, for which a CoFe/NiFe composite has commonly been used [Katine and Fullerton, 2008]. The metallic spacer layer between the free layer and reference layer is Cu. The reference layer may then be Co/Ru/Co or CoFe/Ru/CoFe stack with a Ru interlayer thickness chosen to achieve antiferromagnetic coupling. The given reference layer stack, when interfaced with Cu, provides good transport properties for a good GMR
Figure 12.2: Spin valve in (a) parallel and (b) antiparallel state. Due to spin-dependent scattering, the electrical resistance is greater when the device is in the antiparallel state.

response, while at the same time, is to a large extent magnetostatically invisible (being a synthetic antiferromagnet), and so does not interfere with the response of the free layer. An antiferromagnetic layer, such as IrMn, is used to pin the magnetization of the reference stack along the reference direction.

GMR read heads helped significantly extend magnetic recording areal densities. Further increases in density came with the transition from current-in-plane (CIP) GMR read heads to current-perpendicular-to-plane (CPP) TMR read heads. The main structural and material differences between the two sensor types is that in CPP TMR heads the spacer between the free layer and reference layer is insulating (e.g., MgO) instead of metallic, and the leads are connected to the multilayer stack directly from the top and bottom, rather than at the edges (Fig. 12.1b). As before, the relative alignment of the free layer and the reference layer determines the voltage output, which is used to infer the recorded magnetization states occurring beneath the read head. Due to the significant difference in the reflection and transmission coefficients between the two spin species in the magnetic tunnel junctions (MTJs), the MR efficiency is about two orders of magnitude greater than for all-metallic spin valves.

Though the introduction of CPP TMR read heads resulted in improved readout resolution and provided a path to greater areal densities, further scaling down of TMR sensors will ultimately result in excessive junction resistances due to the reduced MTJ area, which will limit readback rates. Consequently, CPP GMR read sensors with much lower resistances are being considered to overcome this problem [Katine and Fullerton, 2008]. The MR efficiency of CPP GMR sensors will be inherently lower than that of
their TMR counterparts, which will necessitate the use of higher current densities to
achieve the required signal resolution. However, too large current densities can lead to
spin transfer torque (STT) induced modes in the free layer, which may act as a new
source of output noise in CPP GMR.

Several solutions have been proposed to mitigate this effect. One solution involves
using materials with a high RA-product and good transport properties to improve signal
strength. Modifying the free layer composition to obtain greater damping can help quench
STT-induced magnetization dynamics, without degrading the MR response. A dual spin
valve design has been proposed in which the free layer is sandwiched between two equally
oriented reference layers so that angular momentum deposited onto the free layer across
one interface is counterbalanced by the angular momentum deposited onto the free layer
across the other interface. The drawback of such a design is increased separation between
the shields (due to the extra layers in the dual-MTJ stack), which places a limit on the
achievable down-track areal density. Nonlocal spin valves [Jedema et al., 2001] are being
considered for reducing shield-to-shield spacing. An example of the media design that
provides a pathway to improved readback response when the shield gap is insufficiently
narrow is described in section 11.5. A detailed review of read head technology and spin
torque applications can be found in [Katine and Fullerton, 2008].

12.1.2 Magnetic Random Access Memory

Magnetic random access memory (MRAM) is a developing memory technology
integratable with CMOS circuitry that seeks to combine nonvolatility with high data
rates, low power consumption, and endurance. In anticipation of materials and design
solutions, MRAM is regarded as a viable candidate for assuming the role of a universal
memory platform for common, industrial, and military applications. In this subsection we
outline the evolutionary trend in MRAM technology, beginning with a description of first-
generation MRAM, followed by an analysis of the improved STT-based MRAM design
and the challenges that remain to be overcome in order for it to supersede established
memory technologies such as SRAM, DRAM, and flash.

Field-switched MRAM was the first commercialized MRAM technology, marketed
for applications in harsh environments, e.g., on board airplanes, satellites, etc. The
field-switched MRAM architecture consists of an array of patterned memory elements
located at cross points between perpendicularly running leads known as the word and
Figure 12.3: Cross-point architecture of magnetic random access memory.

bit lines (Fig. 12.3). The memory elements are MTJs similar to those used in CPP TMR read heads (section 12.1.1), save that the free layers in MRAM are designed to have sufficient uniaxial anisotropy to provide the necessary thermal stability to render the application nonvolatile. This is conventionally done by patterning the MTJs into elliptical pillars so that shape anisotropy provides the needed bistability.

One way to write a bit in field-switched MRAM is to concurrently send two current pulses, one down the word line and one down the bit line, at whose cross point is the memory element that is to be addressed. The Oersted fields from the two pulses superimpose at the cross point of the word and bit line, resulting in a net field strong enough to switch the selected bit. One disadvantage with this scheme is that some of the remaining bits which are half-selected may also switch due to the switching field distribution originating from material and structural fluctuations which are especially prominent for small MTJ feature sizes.

Toggle MRAM was introduced to mitigate this effect. In toggle writing, the free layer is a weakly coupled Co/Ru/Co synthetic antiferromagnet, and the currents are passed down the word and bit lines as pulses with a phase offset, as plotted in Fig. 12.4c. Since the Oersted fields from the word line and bit line are orthogonal to each other, the net field executes a rotation as the currents are pulsed (Fig. 12.4b). The response of the magnetization of the Co/Ru/Co free layer is to cant in the direction of the external field, so that rotation in the external field results in a rotation of the canted magnetizations in
the two antiferromagnetically coupled Co layers, as depicted in Fig. 12.4b. The toggle writing scheme has the advantage of writing a bit at the cross point of the word and bit line with minimal disturbance to the memory elements lying along the two lines away from their intersection. The result is reduced bit-error rates.

Retrieving a bit in field-switched MRAM involves sending a small current down the bit line and reading the voltage difference across the MTJ between the bit line and a bypass line [Katine and Fullerton, 2008]. Depending whether the free layer and reference layer magnetizations are mutually parallel or antiparallel, the MTJ will be in the low-resistance or high-resistance state on account of the TMR effect, and the voltage amplitude will correspondingly reflect the state of the memory element.

In field-switched MRAM, spintronics plays a part in only the readback process. In the newest generation MRAM technology, spintronics has a role in both the reading and writing of the bits. A current is used to read the bits through the TMR effect, as before, but this time the STT effect is employed for the purpose of writing. Fig. 12.5 illustrates the switching of an elliptical MRAM element with electric current. The great advantage of current-switched MRAM is that memory elements can be placed closer together without affecting write margins owing to the local nature of the STT effect as opposed to the long-range action of the Oersted fields. This further reduces power consumption and allows for a simplified and more scalable MRAM cell [Katine and Fullerton, 2008].
Figure 12.5: Current-induced switching of the free layer in an STT-MRAM element. Plots show the three spatial components of the average MRAM element magnetization during the reversal process.

Much effort is under way to reduce the current density required to switch the MTJ memory elements. Achieving low switching current densities is not only important to decrease power consumption, but also to ensure device durability, and to allow a single transistor to address a bit so as to maximize efficiency and density. The expression relating the critical writing current to the material and structural properties of the free layer in an in-plane MRAM MTJ memory element (Fig. 12.6a), in the macrospin approximation at zero temperature, is

$$I_{C0} = \frac{2e}{\hbar} \frac{\alpha}{\eta(\theta)p} M_s V \left( H_{K||} + 2\pi M_s \right),$$

(12.1)

where $H_{K||}$ is the in-plane magnetocrystalline anisotropy field, $M_s$ is the saturation magnetization, $V$ is the free layer volume, $\alpha$ is the damping constant, $p$ is the current polarization, $\eta(\theta)$ specifies the angular dependence of the STT efficiency, and $e$ and $\hbar$ are the fundamental charge and reduced Planck constant, respectively.
Figure 12.6: (a) In-plane and (b) all-perpendicular MRAM element consisting of (from bottom to top): seed layer, antiferromagnetic layer, pinned layer (stabilized by the antiferromagnetic layer), reference layer (antiferromagnetically coupled to the pinned layer), tunnel barrier, free layer, and capping layer.

We can see that reducing $\alpha$ and increasing the $\eta(\theta)p$ product results in reduced $I_{C0}$, suggesting that materials engineering will play a major role in making STT MRAM a viable storage solution at high bit densities. Since the energy barrier separating the two stable states of the free layer is given by $E_b = M_s V H_{K\parallel}/2$, which, for thermal stability requirements has to satisfy the condition $E_b \geq 50k_B T$, we are not at liberty to adjust this term to achieve a lower current threshold. However, the shape anisotropy field $2\pi M_s$, which does not enter into the stability, can be partially balanced by an out-of-plane anisotropy contribution $H_{K\perp}$, that can be introduced to the free layer, to result in a reduced critical current

$$I_{C0} = \frac{2e}{\hbar} \frac{2\alpha}{\eta(\theta)p} M_s V \left( H_{K\parallel} + 2\pi M_s - \frac{H_{K\perp}}{2} \right).$$  \hspace{1cm} (12.2)

The closer $2\pi M_s - H_{K\perp}/2$ is to zero, the lower is $I_{C0}$.

It has been demonstrated that switching efficiency is greater in perpendicular magnetic anisotropy spin valves [Mangin et al., 2006]. The magnetization goes out-of-plane when $H_{K\parallel} = 0$, $H_{K\perp} > 4\pi M_s$ (Fig. 12.6b). In this case, the threshold current is directly proportional to the energy barrier,

$$I_{C0} = \frac{2e}{\hbar} \frac{2\alpha}{\eta(\theta)p} E_b,$$  \hspace{1cm} (12.3)

where $E_b = (M_s V/2)(H_{K\perp} - 4\pi M_s) = (M_s V/2) H_{K\perp}^{\text{eff}}$. It has been recently shown that CoFeB/MgO/CoFeB MTJs can exhibit perpendicular magnetic anisotropy, and, unlike
previously explored material systems for perpendicular MTJs, the CoFeB/MgO/CoFeB perpendicular system achieves low switching currents, high TMR ratios, and high thermal stability, simultaneously [Ikeda et al., 2010]. For a 40 nm diameter MTJ, the critical currents density for switching at room temperature for the parallel-to-antiparallel and antiparallel-to-parallel transition was $J_{C}^{P\rightarrow AP} = 1 \times 10^6$ A/cm$^2$ and $J_{C}^{AP\rightarrow P} = 4 \times 10^6$ A/cm$^2$, respectively, corresponding to switching times of $\tau_{sw} \approx 1.0$ s. The same samples had an MR ratio over 100% and an extracted thermal stability factor $E_{b}/k_{B}T \gtrsim 40$. Though very encouraging, these values need to be further improved for STT-MRAM to become a competitive memory solution for a broad range of applications [Sato et al., 2011, Gajek et al., 2012, Sun et al., 2012].

We now consider the relationship between critical current densities, switching rates, switching probability, and temperature to better understand the path to optimization for safe operating margins, low power consumption, high operating speeds, and reduced bit-error rates. Analytical models and experiments show that the average rate of switching $\tau_{av}$ in perpendicular magnetic anisotropy nanopillars under spin-polarized currents for short times, during which thermal effects play an insignificant role, is inversely proportional to the difference between the applied and critical currents [Bedau et al., 2010a, Bedau et al., 2010b]

$$\tau_{av}^{-1} = A (I - I_{C0}) .$$  \hspace{1cm} (12.4)

For long timescales, from first principles and Fokker-Planck calculations, the switching rate for thermally-assisted reversal under the influence of spin transfer torque is given as [Bedau et al., 2010b]

$$\tau_{av} = \tau_{0} \exp \left[ \left( 1 - \frac{I}{I_{C0}} \right) \frac{E_{b}}{k_{B}T} \right],$$  \hspace{1cm} (12.5)

which can be recognized as a modified Arrhenius-Neél law with the exponential prefactor $(1 - I/I_{C0})$ being understood as defining the effective temperature $T_{eff} = (1 - I/I_{C0})^{-1} T_{b}$, or the effective barrier $E_{b}^{eff} = (1 - I/I_{C0}) E_{b}$. The former interpretation is more sound in that the STT effect dynamically pumps (or dissipates) energy and cannot be cast in the form of a potential the same way as anisotropy, exchange, magnetostatic, and Zeeman interactions. The latter interpretation however mirrors the relational dependence of the energy barrier on the applied field, indicating that the field and current may at times be conveniently treated on the same footing.

Considering then expressions (12.4) and (12.5), and noticing that the switching time for current densities of around $1 \times 10^6$ A/cm$^2$ was on the order of 1 s in the original
perpendicular CoFeB/MgO/CoFeB MTJ demonstration [Ikeda et al., 2010], it can be concluded that for sub-microsecond reversal times the magnitude of the current would have to be at least an order of magnitude higher. For STT MRAM to become competitive with leading memory technologies, the switching times will have to be reduced to within 1–10 ns. The currents that would be required for such ultrafast switching dynamics would damage the considered CoFeB/MgO/CoFeB systems.

Even if lower switching times can be afforded for a given application, the switching current distributions due to MTJ nonuniformity and thermal fluctuations may impose a still high current requirement for reliable operation. The reported probability for switching in the short time scale regime is

\[
P = \exp \left\{ -4 \frac{E_b}{k_B T} \exp \left[ \frac{2}{\tau_D} \left( 1 - \frac{I}{I_{C0}} \right) \right] \right\},
\]  

and for switching in the long time scale regime

\[
P = 1 - \exp \left\{ -\frac{\tau}{\tau_0} \exp \left[ - \left( 1 - \frac{I}{I_{C0}} \right) \frac{E_b}{k_B T} \right] \right\},
\]

where \( \tau \) is the write current pulse duration, \( \tau_D = (\alpha \gamma H_K)^{-1} \), and \( H_K \) is the effective anisotropy field [Bedau et al., 2010b].

Relations (12.6) and (12.7) illustrate the tradeoff between the switching probability, switching time, and write-current magnitude. Depending on the specific application, it may be possible to relax one criterion in favor of another. However, in the effort to make STT MRAM a more competitive technology, and potentially the universal memory solution, it will be necessary to ensure device durability, operational reliability, low power consumption, enhanced data rates, and high-density integrateability with CMOS technology, all at the same time. This implies a \( P \) exceptionally close to unity, \( \tau < 10 \) ns, and a write current \( I_{\text{write}} \) which does not exceed the maximum output of a single transistor.

In addition to investigating advanced materials solutions to lower \( I_{C0} \), exploring design solutions will be important as well. A dual-tunnel spin valve has been proposed to reduce \( I_{C0} \) by allowing for deposition of spin angular momentum on both sides of the free layer. In contrast to the dual GMR readback sensor proposed for hard disk drives (section 12.1.1) where the magnetizations of the two reference layers were aligned in order to result in spin torque cancellation, in the dual-tunnel spin valve the magnetizations of the reference layers are antiparallel so as to result in an enhanced net spin transfer torque effect. This leads to a significant reduction in \( I_{C0} \), and also lessens the asymmetry
in the switching currents reflected in the parameter $\eta(\theta)$, which leads to the discrepancy $I^P\rightarrow AP \neq I^{AP}\rightarrow P$. Designs exploring the relative angles between the reference layer and free layer, as well as combinations of anisotropy and exchange bias contributions, were recently proposed to decrease operational currents or increase write rates. Care will have to be taken in the future design of STT MRAM in order to ensure that the read current amplitude does not approach the threshold for STT-induced reversal. In this respect, careful material and design considerations will be necessary to ensure that the write margins and the signal-to-noise ratio (SNR) do not give rise to a significant tradeoff. For achieving high memory densities (low critical currents and high energy barriers), it will additionally be necessary to avert the positive correlation between $I_C$ and $E_b$ observed for perpendicular magnetic anisotropy materials [Ikeda et al., 2010, Pal et al., 2011, Fujita et al., 2008, Mizukami et al., 2010, Sajitha et al., 2010, Beaujour et al., 2009]. Section 12.2 presents a composite free layer spin valve design which lowers $I_C$, reduces the coupling between $I_C$ and $E_b$, and provides a means toward low effective damping at high $H_K$, important for scaling toward high capacities.

12.1.3 Spin Valve Logic

Since spin valves are used as the digital storage elements in MRAM for encoding bits 1 and 0, it is only natural to consider them for use in binary logic [Black and Das, 2000]. The truth values 1 and 0 are encoded by the two possible magnetization configurations of the spin valve (parallel and antiparallel). Just as in MRAM, readout is achieved by exploiting the magnetoresistance effect (section 12.1.1). Considering that a spin valve can be switched from the parallel to the antiparallel state, and vice versa, by external stimulus, only if the stimulus strength exceeds a certain threshold, it becomes clear that Boolean operations are achievable.

To demonstrate how a spin valve can be used to perform Boolean operations, we refer to a particular design [Ney et al., 2003, Pampuch et al., 2004], shown in Fig. 12.7a. In this design three independent current carrying field lines A, B, and C are used to drive operation. In the immediate vicinity of these wires is an MTJ consisting of a magnetically hard (bottom) and soft (top) layer, separated by a thin nonmagnetic layer. The magnetic layers are of in-plane magnetic anisotropy.

The current lines, A, B, and C are used to convey logical input to the MTJ. The value of the logical input is determined by the sense of the current in the current lines.
Following the convention in [Pampuch et al., 2004], we associate a logical 1 to the current sense resulting in an Oersted field through the MTJ oriented to the right, and a logical 0 to the opposite current sense (Fig. 12.7a). Wires A and B are assumed to carry current amplitudes $I_A$ and $I_B$, resulting in Oersted fields at the MTJ, of amplitudes $H_A$ and $H_B$, each greater than the switching field of the top soft layer $H_{sw}^{soft}$. The magnetic field from wire C is assumed to be greater than the switching field of the bottom hard layer ($H_C > H_{sw}^{hard}$). For proper functioning, it is important that $H_A + H_B < H_{sw}^{hard}$ so that input lines A and B do not influence hard layer switching.

Subscribing to the declared convention regarding the logical values of the input wires, and assigning a logical 1 to the low resistance state of the MTJ, and a logical 0 to the high resistance state, all primitive logic functions can be demonstrated using the setup as described. The MTJ, with the three input wires, can thus be regarded as a reprogrammable logic element. Preconfiguring the MTJ to the antiparallel state with the hard layer magnetized to the right, one prepares the gate for the logical AND operation (Fig. 12.7b). Reversing the soft layer magnetization to set the MTJ in the parallel (right-oriented) state reconfigures the gate to perform the logical OR operation (Fig. 12.7c). The gate can be preset to perform the desired logical function by first orienting the hard layer in the chosen direction via wire C. The field from wire C inevitably orients the soft layer along the same selected direction. The soft layer can be addressed subsequently via lines A and B, without disturbing the hard layer. The sequential two-step procedure outlined here can be used to achieve all possible MTJ configurations. The overhead cost...
in time and power resulting from preconfiguring gate functionality is small, considering the derived benefits, as stressed below.

Once the MTJ is preconfigured for a specific function, pulses representing the input truth values can be sent down field lines A and B for processing. The response of the soft layer to the input pulses is reflected in the MTJ’s output resistance state. Truth tables in Figs. 12.7b,c show the output values C for different combinations of input values A and B for the AND and OR gates.

Simply reversing the orientation of the hard layer prior to operation inverts the gate functionality, resulting in the negated AND (NAND) and negated OR (NOR) gates. Logical negation (NOT), alone, is achieved by presetting the hard layer to point left, and equating the logical inputs A and B to serve as one input. The IDENTITY operation is realized by presetting the hard layer in the contrary direction. If wire C, which presets the hard layer, is used to convey the second logical input, then the gate effectively performs the logical exclusive NOR (XNOR) operation. The XNOR gate becomes a XOR gate if the second input is passed as a negation through wire C. The logically reversible controlled NOT (CN) and the controlled controlled NOT (CCN) gates can be achieved on same principles [Pampuch et al., 2004].

We observe that numerous logical operations can be performed employing the same spin valve logic unit design. While the realization of the NOT, NAND or NOR, AND or OR, and XOR gates using CMOS requires the use of two, four, six, and \(\sim 10\)–16 transistors, respectively, the same functionality can be accomplished with a single magnetoresistive element and accompanying input field lines. Since both layers, which together define the resistance state of the magnetoresistive element, are addressable by the input field lines, the logic is dynamically reconfigurable. This implies that the functionality of logic circuits based on spin valves can be morphed on-the-fly, thus enabling task-specific processing optimization, which stands in contrast to CMOS logic architecture where circuit functionality is predominantly hardwired.

Even in lookup table-based field programmable logic arrays (FPGAs), only partial reconfiguration is offered, based on programmable logic blocks and switchable interconnects [Black and Das, 2000]. The use of FPGA is typically limited to prototyping, due to the low density and performance resulting from particular wiring and related expenditures. The communication between the local or remote memory and logic blocks further slows operation. A big advantage of spin valve logic is that it is nonvolatile which
eliminates the need to transfer the output of the logical operation to memory, i.e., the magneto resistive element can indefinitely store the output itself, which can be readily accessed via the sense line as needed.

The ability to both process and store, as offered by spin valve logic architecture, implicates the possibility of asynchronous operation, i.e., multiple clocking stages, enabling gates to perform parallel computation. The simplicity of spin valve gates, inherent nonvolatility, and reconfigurability provide a path toward ultra-parallelized processing architectures with on-the-fly task-specific optimization, which could potentially lead to orders of magnitude improvement in computational efficiency over CMOS-based logic architectures.

While the reconfigurability of spin valves offers great possibilities for high performance logic design, concatenability must be considered for the implementation of more complex circuits. Since the gates presented so far consist of a spin valve and three input field lines, depending on the particular arrangement, not all lines may be independent. For instance, in MRAM-like architecture, each bit in the word line is shared by many magneto resistive elements in a row. For logic applications, spin valves sharing a common input field line cannot be passed independent input through the line, which reduces the level of reconfigurability of a logic circuit. Incorporating more field lines to allow greater reconfigurability would have the disadvantages of spiked production cost, exaggerated implementation complexity, and diminished gate density. Alternative solutions have been proposed.

In one design, the three field line gate of [Ney et al., 2003] has been reduced to a one field line gate with added CMOS circuitry [Lee et al., 2007b]. The modified gate allows for three input values as before, but now the input values, through the added circuitry, prescribe not only the current direction, but also the amplitude of the current passing through the single field line. The design was shown to perform all the logic operations of the three-field line gate in an essentially equivalent manner based on the input. While the added CMOS circuitry increases architectural complexity, it should allow for greater freedom of integration and reconfigurability, as a single field line drives operation, for which reason the number of spin valves sharing a common field line is reduced. The design concept also eliminates the two-step gate preconfiguration sequence needed for functionality selection, which simplifies operation.

Several designs of spin valve logic whose operation involves the use of spin polarized
currents have also been proposed. The local nature of spin transfer torques, in contrast to Oersted fields, is advantageous in terms of scaling and power consumption. A design employing circuitry similar to that of the single field line gate [Lee et al., 2007b] could be used to drive current of different amplitudes directly through a spin valve to effect the reversal of the free layers. A majority gate, involving four magnetoresistive elements, in which the resistance states of the first three elements encode the logical input has also been proposed [Lyle et al., 2010a, Lyle et al., 2011]. The three input elements are connected in parallel (share a common top and bottom electrode), and an output element is connected in series (shares a common bottom electrode) with the rest of the gate elements. The resistance states of the three input spin valves determine whether the voltage drop across the output spin valve is sufficient to induce reversal.

Another means to achieve direct communication between successive magnetoresistive elements is through the use of magnetic interconnects [Lyle et al., 2010b, Yao et al., 2012]. The interconnects serve as conduits for domain wall propagation, and separate input and output elements. Notches at the center of the interconnects serve as pinning potentials for the domain walls and provide stability. The spin transfer torque effect is used to depin and drive domain walls to and from the magnetoresistive elements. An efficient arithmetic logic unit (ALU) based on such a design was recently demonstrated, consisting of 20 MTJs and two amplifiers [Yao et al., 2012]. The demonstrated ALUs can be used to perform highly parallelized computations for video processing applications. Other three terminal DW-switchable spin valve logic devices have also been proposed and shown to improve operational speeds due to the separation of the read and write paths [Zhu et al., 2011].

In summary, we have considered several proposed logic gate implementations based on spin valves. The prospects of spin valve logic will in great part depend on the success of MRAM technology. Once key technological requirements for the mass-commercialization of MRAM are met, such as low current operation, high switching rates, high TMR (or GMR) ratio, ample thermal stability, and small feature size, the primary challenges facing spin valve logic will be reduced to circuit design and implementation. The great difference between spin valve logic and MRAM is that the latter features an economical crosspoint architecture, unsuited for reconfigurable Boolean processing. Highly reconfigurable spin valve logic circuit implementations are imperative to allow on-the-fly task-specific circuit optimization for increased computational performance competitive with CMOS
technology. Direct communication between spin valves is important for reducing delays due to information being passed through intermediary sense amplifiers, and for helping reduce costs through reductions in accessory CMOS components, gate footprints, and power consumption. The separation of the write and read paths in logic units may lead to further gains in operating speeds. Integration with CMOS will factor in the overall computational efficiency of spin valve logic circuits, as well. Integratability is the topic of significant ongoing investigation, which encompasses theoretical work, micromagnetic and HSPICE simulations, and experimental work [Prenat et al., 2009, Matsunaga et al., 2009, Ohno et al., 2010]. In light of the recent progress in MRAM technology, including the demonstration of CoFeB/MgO/CoFeB MTJs with high PMA and TMR, and ongoing investigations into design solutions and integratability with semiconductor technology, a nonvolatile, reconfigurable, and massively parallel magnetic logic architecture integrated with CMOS could emerge in due course.

12.1.4 Spin-Torque Nanooscillators

Spin transfer torques (STTs) can be used to achieve steady-state magnetization precession in nanoscale devices having geometries similar to the spin valves discussed in sections 12.1.2 and 12.1.3. Sustained precession is the result of compensation between magnetization damping and spin injection. Devices tailored to operate in such a steady-state regime are called spin-torque nanooscillators (STNOs). They are of technological interest because the precessional frequency is in the GHz range and it can be easily tuned by current and field biases. The devices can operate over a wide range of temperatures and sport nanoscale dimensions. Several STNOs can be coupled to each other by spin waves [Kaka et al., 2005, Mancoff et al., 2005], or coupled to external DC or microwave signals [Tsoi et al., 2000, Rippard et al., 2005, Georges et al., 2008, Slavin and Tiberkevich, 2009, Dussaux et al., 2010a] to achieve diverse dynamical responses. STNOs can be used for microwave-assisted magnetic recording (sections 9.1.4, 11.2.4–11.2.6) to pump energy to assist the switching of high anisotropy bits. Efficient implementation of STNOs in magnetic recording heads is an active area of research among specialists in industry and academia [Matsubara et al., 2011, Zhu and Wang, 2010]. Other applications of STNOs include signal transmission in telecommunication, frequency stabilization, and clocking. Since the angle/amplitude of oscillations can be electrically detected by the GMR or TMR effects (section 12.1.1), STNOs can also be used in the response regime as sensors
Figure 12.8: Curves indicating combinations of current and field amplitude and direction resulting in steady-state precession of a simplified all-perpendicular spin valve. Plots show the magnitude of the torque due to the field (blue curves) and current (green curve) as a function of magnetization polar angle. Plots (a)–(c) assume an all-metallic spin valve with asymmetric spin transfer torque efficiency, while plot (d) assumes a magnetic tunnel junction with symmetric spin transfer torque efficiency.

of diverse utility. The drive/response regimes of STNOs, current/frequency modulating capability, hysteretic proclivity, and integrability, could enable their employment as dynamic processing components of advanced neuromorphic circuits and autonomous devices. Irradiation hardness and compatibility of STNOs with other systems and technologies suggest their usefulness for military applications.

The response of a STNO to an applied current and field can greatly vary depending on the current and field bias intensity and direction, size of the device, system geometry, configuration, materials choices, and ambient temperature. The geometry and materials determine the magnetic anisotropy direction and energy density of the STNOs and further
define the STT efficiency and its angular dependence (section 4.1). To illustrate how some of these properties influence dynamical response, we consider a simplified MR stack consisting of a free layer and fixed perpendicular polarizer, subject to a current and a vertically applied field (Fig. 12.8). Neglecting the out-of-plain contribution (section 4.1.2), the spin transfer torque on the free layer may be expressed as

$$\tau_{\text{STT}} = \sigma \eta(\theta) \frac{1}{t_f} \frac{\hbar J}{2} \sin \theta \hat{\theta},$$

(12.8)

where \(\sin \theta \hat{\theta} = \hat{m} \times \hat{m} \times \hat{z}\) (see 4.1), \(\theta\) is the angle between the vertical direction and the magnetization, \(t_f\) is the thickness of the free layer, \(\sigma = \pm 1\) defines the magnetization orientation of the polarizing layer (along \(\hat{z}\)), and \(\eta(\theta)\) is the angular dependence determined by device-dependent parameters \(q^+, q^-, A, B\) as [Xiao et al., 2005]

$$\eta(\theta) = \frac{q^+}{A + B \cos \theta} + \frac{q^-}{A - B \cos \theta}.$$ 

(12.9)
The damping torque due to the applied field \( \tau_a^\alpha = -\frac{\gamma_\alpha}{1+\alpha^2} \hat{m} \times \hat{m} \times H_a \) (see (2.4)) may be rewritten as

\[
\tau_a^\alpha = \frac{\gamma_\alpha}{1+\alpha^2} H_a \sin \theta \hat{\theta} .
\] (12.10)

If the free layer of the device has a zero magnetocrystalline anisotropy, and magnetostatic effects are small compared to the influence of the external field, steady-state precession can be expected at angles \( \theta_{SSP} \) for which \( \tau_{STT}(\theta_{SSP}) + \tau_a^\alpha(\theta_{SSP}) = 0 \) holds (excluding trivial solutions \( \theta = 0 \) and \( \theta = \pi/2 \), corresponding to static states). Clearly, steady-state solutions are absent for specific combinations of device-dependent parameters and applied field magnitudes (Figs. 12.8c,d). Moreover, Fig. 12.8d illustrates that a steady-state solution is altogether absent for any applied field \( H_a \), when \( \eta(\theta) = \eta_0 \) (a flatter \( \eta(\theta) \) often resembles MTJs). In other cases, solutions exist only for \( \theta > \pi/2 \) (or \( \theta < \pi/2 \)); Figs. 12.8a,b. Steady-state precession of the described STNO is illustrated in Fig. 12.9.

The stability of the solution at \( \theta_{SSP} \) depends on the relative orientations (or sign) of the applied field \( H_a \), electric current density \( J \), and magnetization direction of the polarizing layer \( \sigma \). This is illustrated by the arrows displayed on the curves in Figs. 12.8a,b. The arrows signify the direction in which the torques tend to change the angle \( \theta \), whereas the curve altitude relates the torque magnitude. The angles formed by the intersecting \( \tau_{STT} \) and \( \tau_a^\alpha \) curves significantly bear on the frequency spectrum of the STNO [Russek et al., 2010]. The less similar the two curves are in magnitude in the vicinity of the intersection, the less susceptible is the STNO to thermally induced broadening of the spectral linewidth. Narrow linewidths are especially important for enhancing STNO phase locking capability, but are also a generally sought characteristic for all STNO applications. Notice that while the STNO model depicted in the inserts of Fig. 12.8 can be used to generate an oscillating microwave field, a reference layer with in-plane magnetization must be included in the multilayer stack if the steady-state precession is to be converted to an oscillating voltage output.

While the illustrated STNO exhibits only three states (two static states corresponding to magnetization oriented upwards or downwards along \( \hat{z} \), and a dynamical state where the magnetization undergoes precession at some fixed cone angle \( \theta_{SSP} \)), STNOs of other geometries (Fig. 12.10), where the extent of the magnetic layers may differ, and where the applied fields and magnetic anisotropies of the polarizing and free layers may be oriented differently, can exhibit a variety of dynamical modes. Dynamical responses may be further affected by additional free layers or polarizers and other magnetic layers that
Figure 12.10: Spin-torque nanooscillators: (a) pillar oscillator with in-plane magnetic anisotropy; (b) oscillator with extended in-plane polarizing layer and confined perpendicular free layer; (c) in-plane oscillator with extended polarizing and free layers with point contact; (d) patterned all-perpendicular pillar oscillator.

can be introduced to the stack, and also by modulation of applied biases. Considering that STNOs are made up of highly magnetoresistive multilayers, and that often the extent of these multilayers exceeds the critical length below which the layers behave as macrospins, a wide range of possible modes may be expected (see Fig. 12.11, for example). Material and structural distributions can further lead to variations in the dynamical response. Some of the studied dynamical behaviors include in-plane and out-of-plane modes in STNOs, edge modes, vortex oscillations in point contact geometries, vortex-vortex and vortex-antivortex paring, spin wave generation, phase locking, and mode hopping.

Despite recent success in demonstrating STNO functionality in devices of various geometries and configurations [Kaka et al., 2005, Mancoff et al., 2005, Rippard et al., 2005, Boulle et al., 2007, Houssameddine et al., 2007, Pribiag et al., 2007, Georges et al., 2008, Dussaux et al., 2010b, Deac et al., 2008], further strides will be needed before STNOs can enter a broader class of applications. Specifically, the output power and frequency should be significantly enhanced, the linewidths narrowed, and materials selection and fabrication process optimized to limit device variability. These challenges in part require systems and materials solutions, many of which have recently been proposed. The output power, for example, can be enhanced by synchronizing multiple STNOs, and extracting the signals while preserving the phase relationships [Russek et al., 2010]. Different phase locking methods for different STNO types have been considered and demonstrated [Slavin
and Tiberkevich, 2009]. Frequencies can be enhanced by increasing the applied fields and currents during operation. To avoid having to externally apply fields, additional magnetic layers may be incorporated which exert local effective fields allowing for high-frequency operation. Materials and configuration considerations can help reduce distributions and linewidths. Narrow linewidths can further improve STNO synchronization propensity and help boost output power. Improved patterning capability is important in reducing linewidths, as etch damage can introduce changes in magnetic properties that contribute to response variability. More on STNOs and dedicated research activity can be found in [Russek et al., 2010, Slavin and Tiberkevich, 2009], and references therein.

12.2 All-Perpendicular Composite Spin Valve: Critical Switching Currents, Thermal Stability, and Scaling

12.2.1 Introduction

Key implementation challenges for spin torque applications described in section 12.1 were noted to be high critical currents and power consumption, long switching times or decreased probability of switching at reduced currents, strong coupling between critical currents and stability impacting scalability, and a positive correlation between magnetic anisotropy and damping. In the present section, we present a perpendicular magnetic anisotropy (PMA) spin valve design with composite free layers that helps decouple critical switching current from the energy barrier, increases data rates, provides a pathway to meliorate the correlation between anisotropy and damping, and improves scalability [Yulaev et al., 2011].

Figure 12.11: Example of a highly nonuniform oscillation mode possible in an all-perpendicular STNO with 60 nm diameter.
Figure 12.12: All-perpendicular free bilayer spin valve. The free bilayer consists of a magnetically softer layer (magnetocrystalline anisotropy density $K_u = 6 \times 10^5 \text{ erg/cm}^3$) ferromagnetically exchange coupled to a magnetically harder layer ($K_u = 4 \times 10^6 \text{ erg/cm}^3$). The softer layer is separated from the reference layer by a nonmagnetic spacer. The exchange coupling strength across the spacer is $J = 1 \text{ erg/cm}^2$. The reference layer magnetization is pinned. All layers have a saturation magnetization $M_s = 600 \text{ emu/cm}^3$ and an exchange stiffness $A_{ex} = 1.0 \times 10^{-6} \text{ erg/cm}$. The spin polarization of the electric current is assumed to be $P = 0.35$.

12.2.2 Design Description

The design consists of a reference layer (modeled as a synthetic antiferromagnet with fixed magnetization), a nonmagnetic spacer layer, and a free ferromagnetically exchange coupled bilayer (Fig. 12.12). The free member-layer closer to the reference layer is the magnetically softer of the two member-free layers. Positive current is defined when electrons flow from the reference layer to the free bilayer. The transfer of angular momentum between the reference layer and the neighboring free layer is micromagnetically accounted for through an approach similar to that described in section 4.1. The spin torque interaction between the two free layers can be ignored due to the nature of the coupling interface. The composite spin valve is of cylindrical geometry, with a 40 nm diameter. Material specifications (perpendicular magnetocrystalline anisotropy, saturation magnetization, exchange stiffness, damping, and thickness) are given in the caption of Fig. 12.12.
Figure 12.13: Three spatial components of the magnetization of the harder member free layer (solid blue curves) and softer member free layer (dashed red curves) during the current-induced switching process. The softer layer leads the reversal.

12.2.3 Free Bilayer Dynamics Stimulated by Current Bias

Figure 12.13 demonstrates the typical switching characteristics of the soft/hard free bilayer. The switching was induced by $433 \mu A$ of current flowing from the free layer to the reference layer. The interfacial exchange coupling energy density between the two member free layers was set to $J_{\text{ex}} = 1 \text{ erg/cm}^2$. Similarly as in microwave-assisted magnetization reversal of exchange coupled composite elements [Li et al., 2009b], the softer of the two layers leads the reversal process, being more susceptible to the applied torque due to the absence of a strong restoring anisotropy field. The lateral components of the normalized magnetization ($m_x$ and $m_y$) for the exchange coupled free member-layers are in phase, with the amplitude of oscillations greater for the softer of the two layers, indicating that the softer layer induces motion in the harder layer via the exchange field. We note that, for the case of antiferromagnetic coupling between the softer and harder free member-layers, the in-phase relationship is not preserved, since the preferred direction of precession for the harder layer is counterclockwise to the direction of the anisotropy field,
while the softer layer wants to precess counterclockwise to the exchange field coming from the harder layer, which, for the case of antiferromagnetic coupling, is opposite to the direction of the harder layer anisotropy field. Consequently, the two free layers tend to precess with the opposite cyclicity, a dynamic not supported by the exchange coupling between the two layers. Antiferromagnetic coupling, therefore, has the effect of suppressing reversal dynamics, as observed experimentally in earlier work [Tudosa et al., 2010].

Returning to the present case of ferromagnetic coupling, the perpendicular component ($m_z$) of the softer layer leads reversal, decreasing more rapidly than that of the harder layer. Once $m_z$ of the harder layer has changed polarity ($t \approx 3.4$ ns), the anisotropy field helps to drive it toward $m_z \rightarrow -1$. In this final stage of reversal, the harder layer magnetization precedes that of the softer layer. It can also be seen that when the polarity of $m_z$ changes, so does the cyclicity of precession, as evidenced by the phase change at $t \approx 3.4$ ns.

12.2.4 Critical Current, Switching Field, and Energy Barrier Correlations and Effects of Interlayer Coupling and Pulse Duration

Equation (12.3) describes the coupling between the threshold switching current and the energy barrier separating two stable states in the macrospin approximation. The critical switching field dependence on the barrier was shown to be $H_{sw} \approx \frac{2K}{M_s} = \frac{2E_b}{M_s V}$. Figure 12.14a shows the dependence of critical current, switching field, and energy barrier on the interfacial coupling strength, $J_{ex}$. All values have been normalized to their corresponding values at $J_{ex} \rightarrow \infty$ (single spin regime). As reported elsewhere [Suess, 2007], the barrier dependence on $J_{ex}$ for a soft/hard bilayer is weak. The field and current dependence on $J_{ex}$ is much stronger, consistent with prior observations [Nolan et al., 2011, Bertram and Lengsfield, 2007, Hauet et al., 2009], indicating significant decoupling between the threshold fields/currents and thermal stability, a condition rather promising for reliable operation and scaling of nonvolatile magnetic memories.

Figure 12.14 shows three curves of critical current $I_c$ versus $J_{ex}$ for (a) 20 ns pulses, and (b) 2 ns pulses. The curve with circular plot markers was obtained for zero angular dependence of the STT efficiency, $\eta(\theta) = \eta_0$ (see equation (12.3)). A flat $\eta(\theta)$ more closely represents the STT efficiency of a magnetic tunnel junction (MTJ), and leads to equivalent critical switching current amplitudes for the parallel (low magnetoresistance state) to
Figure 12.14: Critical switching field and current (for the parallel to antiparallel and antiparallel to parallel transitions), and energy barrier as a function of exchange coupling strength between the harder and softer member free layers. All quantities are normalized to values obtained in the strong-coupling limit. Plots (a) and (b) show characteristics for 20 ns and 2 ns current pulses, respectively.

antiparallel (high magnetoresistance state) (P → AP) and the AP → P transitions. For angle sensitive $\eta(\theta) = \frac{q_+}{A+B \cos \theta} + \frac{q_-}{A-B \cos \theta}$ [Xiao et al., 2005], which more closely resembles the STT efficiency across a normal metal spacer, such as in all-metallic spin valves, critical currents for the P → AP and AP → P transitions are significantly different (plotted in Fig 12.14a and b with triangular and diamond markers, respectively). For 20 ns pulses, in Fig. 12.14a, the reduction in critical current for the P → AP and AP → P transition for $J_{ex} = 2$ erg/cm$^2$ is $\sim 40\%$ and $\sim 20\%$, respectively. For 2 ns pulses (Fig.
Figure 12.15: Critical switching current for the free bilayer and reference model for the P → AP and AP → P transitions as a function of current pulse duration.

12.14b), more closely associated with targeted data rates for applications, the reduction for P → AP and AP → P transitions for $J_{ex} = 0.5$ erg/cm$^2$ is $\sim 50\%$ and $\sim 30\%$.

Respectably greater reductions in switching currents should be possible through further optimization of the composite spin valve, involving adjustments in the layer thickness, free layer anisotropy ratio, saturation magnetization, damping, etc. It could also be possible to construct a symmetric dual reference layer, free soft/hard/soft trilayer spin valve to further boost the reduction of threshold currents and help equalize the response for P → AP and AP → P transitions for the case of all-metallic spin valves (section 4.1.1). Considering these possibilities, it is not unreasonable to expect that a $\sim 50\%$ reduction could be brought to a $\sim 90\%$ reduction, which would constitute an order of magnitude improvement in power consumption, and a concomitant improvement in device durability.

Figure 12.15 presents the critical current dependence on pulse duration for the composite spin valve with $J_{ex} = 1$ erg/cm$^2$. The critical currents were again the normalized by their respective values at $J_{ex} = 1$ erg/cm$^2$. The reduction in critical
currents is more pronounced for shorter pulse durations, in agreement with the results presented in Fig. 12.14a and b for 20 ns and 2 ns pulses.

### 12.2.5 Tuning Effective Damping

Another advantage of the proposed composite PMA spin valve design is that the effective damping of the free bilayer can be tuned by adjusting the damping of the softer and harder layers separately. Figure 12.16 demonstrates this property, by showing the critical current dependence on the damping constant of one free member-layer, where the other free member-layer has a fixed damping constant of $\alpha = 0.01$. Though the relationships between the critical current and damping of either or both free member-layers is linear (Fig. 12.16), as indicated by equation (12.3), the dependence is the weakest (shallowest slope) for the case when the damping constant of the harder layer ($\alpha_{\text{hard}}$) is modified. Since a positive correlation between the damping constant and perpendicular magnetocrystalline anisotropy has been observed [Ikeda et al., 2010, Pal et al., 2011, Fujita et al., 2008, Mizukami et al., 2010, Sajitha et al., 2010, Beaujour et al., 2009], the possibility to achieve reduced effective damping in spite of a larger $\alpha_{\text{hard}}$ is a promising pathway to
reduced currents and enhanced scalability.

12.2.6 Concluding Remarks

In summary, we presented a new design concept for a spin valve element envisioned for use in STT MRAM technology. The proposed spin valve includes a free bilayer consisting of the softer magnetic layer ferromagnetically exchange coupled to a magnetically harder layer, with the softer side facing the reference layer. When current is flown through the composite spin-valve structure, the transfer of angular momentum between the reference layer and softer free member-layer results in magnetization dynamics. Placement of the softer layer near the reference layer is advantageous because it allows a greater response of the softer layer to the spin transfer torque than would be achieved for a higher anisotropy layer. As the softer free member-layer precesses under the influence of spin transfer torque, it induces the precession of the harder free member-layer. Under a sufficiently strong current, the precession amplitude increases, and the two layers ultimately reverse. The switching is led by the softer layer, and the threshold currents required for switching are significantly reduced on account of the hard/soft exchange coupling. The presented spin valve design has also been shown to lead to more rapid switching, important for achieving data rates competitive with silicon-based technology. Finally, we have shown the possibility to ameliorate what has been observed to be a positive correlation between the damping constant and anisotropy (and hence switching currents and stability) by tailoring the effective damping of the free bilayer through adjustments in the damping of the softer layer only. This possibility offers a pathway toward reduced operating currents and improved scalability of STT-based MRAM applications.

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13 Domain Wall Devices

Continuing advances in lithography and materials synthesis offer great prospects for a host of devices whose operation relies on the controlled manipulation and propagation of domain walls (DWs) in arrays of nanowires (NWs). After an introduction to DW memory and logic applications, this chapter presents three studies addressing DW motion in magnetically frustrated nanorings [Lubarda et al., 2012b], DW mobility in antiferromagnetically coupled composite NWs [Kuteifan et al., 2012], and DW processing in crosswire architectures [Lubarda et al., 2012c].

13.1 Introduction to Domain Wall-Based Applications

13.1.1 Domain Wall Memory

The most quoted potential application based on the controlled manipulation of DWs is the recently proposed magnetic DW racetrack memory (RM) [Parkin et al., 2008, Hayashi et al., 2008]. The principal building blocks of RM are NWs (i.e., racetracks), which can store arrays of DWs defining a bit pattern (Fig. 13.1). During storage (when not reading or writing bits), the thermal stability of the stored information can be guaranteed through the introduction of equispaced pinning sites along the NWs. The pinning sites can be physical constrictions (notches) or localized variations in material properties. The pinning sites act as potential wells for the DWs with a barrier height $E_b$ that corresponds to the difference in energy between a DW at and away from the pinning center. The depinning time can be estimated from the Arrhenius-Neél law

$$
\tau = \tau_0 e^{-E_b/\kappa_B T}
$$

at zero bias, where $\tau_0^{-1}$ is the attempt frequency. It was shown that the Arrhenius-Neél law can be extended to the more general case of finite field and/or current bias

$$
\tau = \tau_0 \exp \left( \frac{E_{\text{eff}}}{\kappa_B T} \right),
$$

(13.1)
Figure 13.1: Racetrack memory: sequence of domains in a nanowire representing a bit pattern that can be propagated by a current.

where [Burrowes et al., 2010]

$$E_{\text{eff}}^{\text{b}} = E_0^b \left(1 - \frac{H}{H_d}\right)^n - \beta P \frac{\hbar}{e} \frac{\Delta x}{\lambda} I.$$ (13.2)

The dimensionless parameter $\beta$ quantifies the nonadiabatic contribution to the spin transfer torque (section 4.2), $P$ is the spin polarization of the current, $\Delta x/\lambda$ is the ratio of the potential well and DW width, $I$ and $H$ are the current and field biases, $H_d$ is the depinning field at zero current bias, and $E_0^b$ is the barrier height at zero field and current bias. It has been shown that notches and other types of pinning sites can be fabricated to achieve $\tau \geq 10$ years necessary for reliable storage.

In RM, the bits can be written using Oersted fields from a current carrying wire passing in proximity to the racetrack, or by spin transfer torque delivered through a contact element. Reading the bits is accomplished through the TMR effect using an MTJ stray field sensor or an MTJ in contact with the racetrack.

In order to be able to read or write a sequence of bits, it is necessary to be able to shift the DW pattern along the racetrack. For this purpose, current pulses are sent through the NW which result in spin transfer torques that incrementally push the DWs down the racetrack in the direction of the electron flow. RM is therefore a magnetic implementation of a shift register.

Such a memory implementation provides a means towards data rates comparable with those of existing memory technologies. DW velocities of $\sim 100$ m/s have been reproduced in permalloy NWs. Record DW velocities in modified NW structures of $v_{\text{DW}} \approx 1–5$ km/s have been achieved, as well [Lee et al., 2007a, Lewis et al., 2010, Piao et al., 2009, Miron et al., 2011]. The nonvolatility of storage inherent in RM is an important feature that factors in the platform’s absolute operational efficiency, as system power-up and memory loading procedures are circumvented.

Another attractive characteristic of RM is its extendability to three dimensions. Though a significant challenge from a fabrications point of view, the transition from
laterally to vertically oriented arrays of magnetic racetracks could in principle result in a two orders of magnitude increase in storage capacity (assuming a ∼ 100 bits/racetrack density). RM could thus offer storage capacities comparable to rotating disk drives.

However, reliable and efficient writing and reading of a large sequence of bits has not yet been demonstrated. In the original experiment, controllable shifting of only two DWs was achieved. The controlled manipulation of a pattern of ∼ 100 DWs is difficult due to the variations in the material and structural properties in the NWs, including the pinning potentials, which lead to a distribution in depinning currents and DW propagation speeds. This limits the allowable separation between DWs, and hence storage densities.

While original experimental studies focused on Py racetracks, much subsequent investigation was dedicated to high perpendicular magnetic anisotropy (PMA) NWs. Material systems such as (Co/Ni)$_N$ and L1$_0$-phase FePt can support DWs as narrow as 1–10 nm, and provide a means to increased DW storage capacities. Composite NW systems are also investigated as a route to trim distributions, reduce pinning potentials, and lessen non-deterministic behavior. In (Co/Ni)$_N$/CoFeB NWs, the pinning field $H_p$ and threshold current density $J_c$ for DW propagation were shown to be an order of magnitude lower than in (Co/Ni)$_N$ NW alone [Ravelosona et al., 2011].

Generally, reducing the width $w_{NW}$ of a NW increases $H_p$ and $J_c$, because the probability that a random intrinsic pinning potential extends across the entire width of the NW and blocks the DW propagation path becomes greater. The effects of edge roughness are also amplified at reduced NW widths. Further advances in nanoengineering will be key in maximizing scalability of DW-based memories. Micromagnetic studies can assist efforts by helping resolve the contributions of polycrystallinity and grain distributions, edge roughness, and thermal effects to $H_p$ and $J_c$.

Optimizing pinning and depinning processes at artificially introduced pinning sites (notches) will be paramount for reliable and efficient operation of future DW devices. Recent analyses show that the current densities required to depin DWs from pinning potentials sufficiently deep to ensure thermal stability result in significant Joule heating, preventing reliable device operation. Materials solutions can help boost STT efficiency and lower operating currents. One proposal to decrease the threshold current for depinning a DW is to use a periodic current excitation which will pump the DW out of the potential well, in analogy to microwave-assisted field-induced reversal, discussed in section 9.1.4.
A further understanding of the nonadiabatic STT and other torque contributions as well as thermal effects will be necessary before a fully directed optimization of threshold currents, pinning potentials, DW velocities, storage densities, and overall system design can be performed. Knowledge of current-induced depinning and DW motion will not only be important for design of DW memories but also for DW-based logic applications.

13.1.2 Domain Wall Logic

In the previous section we have discussed DW-memory devices. The controlled manipulation and propagation of DWs along networks of NWs can also be used to achieve logic functionality.

In many DW-logic paradigms, a magnetic clocking field is envisioned to drive the computation. Since logic circuits should be able to process a sequence of inputs, the clocking field must be capable of driving an array of domains or DWs down the NW from one computational stage to the next. Achieving simultaneous propagation of multiple DWs in the same direction is, however, not trivial. The application of a magnetic field along the axis of a magnetically soft NW that contains multiple DWs, for example, results in the expansion of domains oriented with the applied field, and ultimate annihilation of domains oriented in the opposite direction. What is sought, rather, is the translation of the entire DW pattern down the NW. To accomplish this, several schemes have been proposed.

One scheme involves cusped NWs and a rotating clocking field [Allwood et al., 2002, Allwood et al., 2005], as illustrated in Fig. 13.2a. The NWs are made of permalloy and the shape anisotropy defines the easy axis for the system, which is always along the NW axis. A rotating clocking field will have the effect of translating the entire domain pattern down the NW, in the direction defined by the handedness of the rotating field. As seen in Fig. 13.2a, after half a cycle, the clocking field shifts the domain pattern one cusp-spacing to the right, inverting the magnetization of each domain. After a full cycle, the pattern is recovered (after two inversions) and displaced two cusped spacings to the right. Assuming that leftward oriented domains represent logical values 1 and the rightward domains represent logical values 0, it can be shown that all of domain patterns can thus be propagated (with the exception of logical sequences 1100 or 0011). Since logic circuitry based on DW motion in cusped NWs can involve bends and loops, the logic states 1 and 0 are defined by the relative orientation of the domain magnetization.
Figure 13.2: Analogous nanowire NOT gate implementations: (a) cusped nanowire with shape anisotropy and a rotating clocking field; (b) perpendicular anisotropy nanofork concatenation and a perpendicular clocking field; (c) nanowire segments with magnetically softer edge exchange coupled antiferromagnetically and a perpendicular clocking field.

with respect to the direction of DW motion [Allwood et al., 2002]. In this interpretation, a logical 1 corresponds to the case when the trailing domain magnetization is along the direction of DW motion, and a logical 0 corresponds to the converse situation.

Cusped magnetic NWs provide a paradigm for constructing a variety of logic circuits. A single cusp represents a NOT gate, and was demonstrated to perform the inversion operation [Allwood et al., 2002]. A bidirectional shift register can be straightforwardly constructed from several NOT gates [O’Brien et al., 2009].

Logical AND, OR, and fanout functionality can also be achieved using Y-shaped NW gates and an elliptically rotating field with a DC offset [Allwood et al., 2005], [Allwood et al., 2006]. Specific operation of Y-shaped gates depends on the relative orientation of the gate and DC offset. Using the developed methodology, and addressing several implementation details, a number of complex logic circuits were shown possible, including multiplexers, flip-flops and latches, and counters [Klein et al., 2008]. For circuits
demonstrated in [Allwood et al., 2002], the achievable operating frequency was estimated to be in the hundreds of MHz. While miniaturization should in principle allow for greater frequency of operation, the effects of NW edge roughness and intrinsic pinning potentials will become more important, as discussed in 13.1.1. Power consumption of the described DW logic was estimated to be three orders of magnitude less than that of CMOS, when energy dissipation per operation is considered, albeit the absolute power performance and heat generation will ultimately depend on the clock structure, which is expected to dominate operational costs. Integrating DW logic with CMOS circuitry is nevertheless estimated to result in reduced overall power consumption.

One concern with the cusped magnetic NWs paradigm is the implementation complexity of a rotating clocking field. An alternative NW logic design has been proposed where operation is based on a perpendicular clocking field. The building block of such a logic design is a two-pronged NW with perpendicular magnetic anisotropy (PMA) bearing the shape of the tuning fork [Jaworowicz et al., 2009]. If such a two-pronged nanofork is concatenated with a straight NW, as shown in Fig. 13.2b, so that the straight NW occupies the inter-tine region of the two-pronged fork without the two touching, one obtains a NOT gate. Because the nanofork and the straight NW are antiferromagnetically coupled through the magnetostatic interaction, after one cycle of the perpendicular clocking field the NOT gate will have performed the inversion operation, assuming that $H_{\text{clock}}^{\text{max}} < H_n < H_{\text{clock}}^{\text{max}} + H_{\text{ms}}$, where $H_{\text{clock}}^{\text{max}}$ is the clocking field amplitude, $H_n$ is the field required to nucleate a domain in the straight NW, and $H_{\text{ms}}$ is the magnitude of the magnetostatic dipolar field in the inter-tine region due to the two-pronged nanofork. The concatenation between the nanofork and the NW acts like the cusp in the previously discussed DW logic design.

Propagation of the domain pattern can be similarly achieved as in cusped NWs by linking several nanoforks together. This is further similar to a chain of antiferromagnetically exchange coupled nanolinks, where each nanolink has an end that is magnetically softer. DW dynamics in structures involving such exchange coupled interfaces in presented in section 13.2.

DW-based logic could also be operated by the spin transfer torque effect, which would further lower power dissipation by doing away with the need for field lines. The principle of current induced propagation of an array of DWs was already discussed in section 13.1.1 in the context of DW memory. Designs utilizing the spinmotive force to
help perform Boolean operations have also been investigated [Barnes et al., 2006]. The success of discussed implementations will ultimately depend on the level of DW control that can be achieved in highly scaled NW networks. To compass the full potential of DW technology, a developed understanding of pinning/depinning processes, influences of pinning potentials, edge roughness, and polycrystallinity, as well as thermal and spin transfer effects is essential.

13.2 Magnetically Frustrated Nanoring

In the present section, we describe a magnetically frustrated nanoring (MFNR) configuration which is formed by introducing antiferromagnetic coupling across an interface orthogonal to the ring’s circumferential direction (Fig. 13.3) [Lubarda et al., 2012b]. Such structures have the unique characteristic that only one itinerant domain wall (DW) can exist in the ring, which does not need to be nucleated or injected into the structure and can never escape making it analogous to a magnetic Möbius strip. Numerical simulations show that the DW in a MFNR can be driven consecutively around the ring with a prescribed cyclicity, and that the frequency of revolutions can be controlled by the applied field. The energy landscapes can be controlled to be flat allowing for low fields of operation or to have a barrier for thermal stability. Potential logic and memory applications of MFNRs are considered.

13.2.1 Motivation and Model Description

Magnetic nanoring structures have been the focus of recent research interest due to their attractiveness for technological applications such as nonvolatile solid-state memory and magnetic logic circuits [Zhu et al., 2000], [Li et al., 2001], [Ross et al., 2006]. Due to their topological characteristics magnetic nanorings can exhibit multiple stable remanent states, controlled by external magnetic fields or currents [Zhu et al., 2000], [Li et al., 2001], [Ross et al., 2006], [Kläui et al., 2003], [Vaz et al., 2007], [Ross et al., 2008], [Chaves-O’Flynn et al., 2009]. Logic gates have also been engineered to perform Boolean operations such as NOT and AND using all-magnetic loop architectures [Imre et al., 2004], [Allwood et al., 2005], [Bowden and Gibson, 2009]. We here model magnetically frustrated nanorings (MFNRs) and describe their magnetic properties, with particular attention to energy landscapes and domain wall (DW) motion.
Figure 13.3: Perpendicular magnetic anisotropy nanoring with AF coupling across interface (colored yellow) located at point A. Due to the magnetic frustration introduced by the AF coupling only one mobile DW with an associated DW energy can exist. The DW can reside either away (Fig. 13.3a, point B) or at the AF interface (Fig. 13.3b, point A).

Magnetic frustration implies a competition between different energy terms so that an energy minimization in one area involves an increase of energy in another. Magnetic frustration is often seen in coupled multilayer systems, due to interfacial disorder [Pierce et al., 1999] or the competition between lateral and vertical exchange [Moser et al., 2003]. In antiferromagnetic materials, it can occur due to the lattice topology, which can prevent all spins from being antiferromagnetically paired [Greedan, 2001]. Molecular structures including flakes and ring-chains have been seen to exhibit geometrically induced frustration as well [Cador et al., 2004]. Magnetic frustration in MFNR presented here is achieved by introducing antiferromagnetic (AF) coupling across an interface orthogonal to the circumferential direction of the ring, as illustrated in Fig. 13.3. As a consequence of such a configuration, the remanent state of the ring involves a DW with an associated DW energy. This is the case regardless of the dominant form of anisotropy (shape or magnetocrystalline). A similar effect would be achieved in a magnetic Môbius strip with a half turn.

For the ring in Fig. 13.3 we have chosen perpendicular magnetocrystalline anisotropy (PMA), so that the magnetization tends toward a vertical orientation. In Fig. 13.3a the magnetization changes orientation twice along the ring, once at the interface at point A due to the AF coupling, and again at some point B in the ring, as a result of system topology. It is important to distinguish between the magnetization reorientation
Figure 13.4: DW configurations near and at the AF interface for (a) relatively strong and (b) weak AF exchange coupling. When AF coupling is large in comparison to the perpendicular anisotropy energy, the DW at the AF interface shows an antiparallel head-to-tail configuration with the DW magnetization largely along the in-plane direction (a). For reduced AF coupling, the perpendicular magnetocrystalline anisotropy tilts the magnetization vertically at the expense of the antiparallel configuration (b).

at point A and point B, because in the former case there is no energy stored in the DW. Only the magnetization reorientation at point B constitutes a DW in the usual sense, with an associated DW energy and mobility. Therefore, the system is fundamentally different from a simple continuous nanoring, as a single DW persists in the system at remanence [Allwood et al., 2005]. By tuning the system parameters, the energy landscape can be made nearly flat, as will be shown below. As a result, the DW can be driven by a weak field and can reside at any location along the MFNR, including the AF interface (Figs. 13.3b and 13.4). Since the system is characterized by a single mobile DW, with an associated DW energy, there is no concern that two DWs may converge and annihilate. The DW can move in any direction, e.g., it can make multiple complete revolutions around the ring with a specified cyclicity, driven by an applied field. Furthermore, the
AF interface eliminates the need for strict synchronization between the external stimulus and DW propagation time due to a tunable DW dwell time at the interface.

### 13.2.2 Energy Calculations

To calculate the energy we use the nudge elastic band method approach (section 6.2). The particular choice of simulation parameters chosen here was to demonstrate the energy landscapes and DW motion in a PMA nanoring. Other parameter values can be used for realization of both perpendicular and in-plane MFNRs. Depending on the strength of AF coupling $J_{AF}$ at the interface, there will be extrema and saddle points in the energy landscape. Figure 13.5a shows that the energy landscape of the nanoring can be tailored by modulating $J_{AF}$ at the AF interface. When the DW is at the AF interface (Fig. 13.3b), the energy of the system significantly decreases as $|J_{AF}|$ is reduced. When $|J_{AF}|$ is increased, the energetic favorability of the DW to reside at the AF interface disappears, as the cost of overcoming the AF coupling energy increases. For appropriate parameters, the MFNR can be tailored so that the energy of the system is nearly independent of the position of the DW along the ring (see red curve with point markers in Fig. 13.5a). The DW can lie away from the AF interface, as in Fig. 13.3a, or at the AF interface, as in Fig. 13.3b, with the system energy equal in both cases.

Figure 13.4a shows the DW configuration near and at the AF interface. The DW structure away and at the interface can be very different without a significant difference in energy (material and structural parameters used for the MFNR in Fig. 13.4a are the same as those used for the MFNR leading to the black curve (diamond plot markers) in Fig. 13.5a. When the DW is at the interface (Fig. 13.4a), the magnetization is largely antiparallel, as expected for AF coupling, with an alignment orthogonal to the ring’s circumferential direction, corresponding to a magnetostatically favorable head-to-tail configuration. For the DW at the interface in the top image of Fig. 13.4a, a large part of the energy is stored in bulk exchange (due to magnetization nonuniformity in the immediate vicinity of the interface) and anisotropy (due to magnetization deviation from the easy axis). However, upon closer inspection, the magnetization across the AF interface is found not perfectly antiparallel, due to competition between different energy terms. The total DW energy therefore includes an important interfacial exchange contribution. When the coupling strength $|J_{AF}|$ is large, even a small departure from antiparallel alignment results in a large interfacial exchange energy. For reduced $|J_{AF}|$, 

Figure 13.5: Energy landscapes for different MFNRs: energy as a function of DW location for three values of (a) AF coupling strength, $J_{AF} = -4, -1, $ and $-0.5 \text{ erg/cm}^2$; (b) saturation magnetization, $M_s = 200, 300, $ and $400 \text{ emu/cm}^3$; and (c) magnetocrystalline anisotropy, $K_u = 1, 2, $ and $3 \text{ Merg/cm}^3$. Remaining material parameters are in (a) $M_s = 225 \text{ emu/cm}^3$, $K_u = 1 \text{ Merg/cm}^3$; (b) $K_u = 1 \text{ erg/cm}^3$, $J_{AF} = -4 \text{ erg/cm}^2$; and (c) $M_s = 200 \text{ emu/cm}^3$, $J_{AF} = -4 \text{ erg/cm}^2$. The intralayer exchange constant, inner ring radius, outer ring radius, and ring thickness in all cases are $A_{ex} = 1.0 \mu\text{erg/cm}$, $R_{in} = 75 \text{ nm}$, $R_{out} = 90 \text{ nm}$, and $t = 12 \text{ nm}$, respectively. The notch depth in part (c) is $7.5 \text{ nm}$ with about $65^\circ$ notch angle. Energy landscapes have been offset for clarity (see discussion in text).
the departure from antiparallel alignment at the AF interface is more prominent (Fig. 13.4b). The MFNR material properties \((M_s, K_u, J_{AF})\) and geometry (inner and outer ring radius, thickness) offer freedom to tailor energy landscapes to be flat, or include energy barriers or wells. For the case of flat energy landscapes, the MFNR can be viewed as a loop containing a single DW that can freely move in either direction throughout the nanoring. The closed loop prevents the DW to escape the structure, which makes the MFNR particularly interesting for long-time studies of stochastic dynamics and DW propagation paths as a function of damping, temperature, DW width, and other parameters [Ravelosona, 2009], [Kläui et al., 2001].

In our study of MFNRs, we are primarily interested in the relative energy landscapes of each ring model which controls the DW mobility, and need not consider common reference (or ground state) energies. In all plots in Fig. 13.5, we have therefore translated the energy landscapes to be within a similar range for clarity. Figure 13.5b illustrates the effect magnetostatic interactions can have on the character of the energy landscapes in MFNRs. The ability to flatten the energy landscape via AF coupling depends on the sample magnetization \(M_s\). For larger \(M_s\) the energy required to bring the DW to the AF interface can be very large (Fig. 13.5b). As the DW approaches the interface, a region of unreversed magnetization (colored red in the insert of Fig. 13.5b) becomes increasingly confined between oppositely oriented segments of the ring, leading to dipolar interactions which can stabilize the magnetization configuration. This is similar to the stabilization of the antiparallel configuration of recorded bits in magnetic recording media due to closed flux lines. This effect leads to the upturn in the energy near the AF coupled region in Fig. 13.5a. This barrier can be modulated by reducing the ring width near the AF interface to compensate the increase in magnetostatic energy with a decrease in anisotropy energy.

Extrema and saddle points can be further introduced to the energy landscape by adding artificial notches which trap the DW in an energy minimum [Burrowes et al., 2010]. Edge roughness and intrinsic pinning sites may then introduce intrinsic distortion to the energy landscape, which can have an additional effect on magnetization dynamics and stability [Kläui et al., 2003]. Figure 13.5c shows the energy landscape for a magnetically frustrated ring containing one artificial notch located at an azimuthal angle of \(\varphi_n = 235^\circ\) with respect to the perpendicular reference line (see inset). The notch spatially confines the DW so that its width (and hence energy) are reduced. The DW, for the parameters used, is a transverse DW. In the example of Fig. 13.5c, a notch size was chosen that
reduces the ring width by a factor of two at the notch center. This approximately lowers
the DW width (the extent of the DW in the direction normal to the ring circumference
at $\varphi_n = 235^\circ$), $w_{DW}$, by a factor of two as well. In a NW with a transverse DW and no
notches, changes in anisotropy $K_u$ result in the broadening (contracting) of the DW due to
the competition between anisotropy energy, $E_{anis}$, and exchange energy, $E_{ex}$, which leads
to the square root dependence of DW surface energy density on anisotropy energy density,
as expressed in $\sigma_{DW} \approx 4\sqrt{K_u A_{ex}}$. However, in the presence of a notch (Fig. 13.5c),
the physical constriction suppresses variations of the DW profile with a changing $K_u$.
With a fixed magnetization profile assumed, the DW energy is linearly proportional to
anisotropy density, $E_{DW} = -K_u \int (\hat{m} \cdot \hat{k})^2 dV + E_{ex}(\hat{m})$, where $\hat{m}$ is the magnetization
unit vector, $\hat{k}$ is the easy axis direction, and integration is over the span of the DW.
Despite the crudeness of the fixed magnetization profile approximation, comparison of the
pinning potentials of the notches $\Delta E$ in Fig. 13.5c for $K_u = 1, 2$ and $3\text{erg/cm}^3$ indicate
indeed a linear dependence on $K_u$, at least for the parameter range and notch dimensions
considered here. We also note that increasing the width or thickness of the nanoring, or
increasing the dimensions of the notch to achieve a greater constriction, would also lead
to a deepening of the pinning potential of the notch, similarly as increasing $K_u$.

### 13.2.3 Magnetization Dynamics

We now illustrate some of the consequences of magnetic frustration on the
response on the nanoring to external stimuli. Figure 13.6 shows the $z$-component of unit
magnetization $m_z = \hat{z} \cdot M/M_s$ versus time (solid black line) in response to an alternating
applied magnetic field $H_a = \hat{z} H_a(t)$ (dotted blue line) in a MFNR with PMA. Simulation
parameters are listed in the caption. The initial configuration of the MFRN is a remanent
state with a DW located at the AF interface. The alternating applied field, with rise and
fall time $\tau_a = 0.5\text{ns}$, period $T_a = 150\text{ns}$, and maximum amplitude $|H_a| = 100\text{Oe}$, drives
the DW from the AF interface along the ring until it spans an angle of $2\pi$, at which point
the DW is back at the AF interface, now with the ring magnetization in the opposite
direction. The DW dwells in this position until the applied field is reversed, upon which
it again departs the AF interface and propagates around the ring once more, repeating
the process for as long as the stimulus is applied.

Several important features should be pointed out. The field driving the DW
motion is $|H_a| = 100\text{Oe}$, which is 50 times smaller than the magnetocrystalline anisotropy
Figure 13.6: The $z$ component of normalized magnetization (solid black line) of a MFRN under a vertically applied field (dashed blue line) as a function of time for a field switching period of $T = 150$ ns. Simulation parameters are $M_s = 200$ emu/cm$^3$, $K_u = 0.5$ erg/cm$^3$, $J_{AF} = -1$ erg/cm$^2$, and damping constant $\alpha = 0.1$. See end of caption to Fig. 13.5 for the remaining material and structural parameters.

Field $H_K = 5$ kOe, and more than 30 times smaller than the coercive field $H_0 = 3.1$ kOe of a similar ring without AF coupling. Because the magnetic frustration necessitates the presence of a DW at all times, DW nucleation is not required. The DW driving field can be made, in principle, arbitrarily small by further tuning the system to obtain a more flat energy landscape. This is accomplished by tuning the system to yield equal energies when the DW is at the AF interface and away from it, as in Fig. 13.5a. If a large $M_s$ is used, dipolar interactions can lead to a rise in energy when the DW is near the interface, as seen in Fig. 13.5b. This can be compensated through magnetostatic coupling to a soft nearby nanomagnet (Fig. 13.7b), which orients itself with the applied field, counterbalancing the dipolar effect. Alternatively, tapering the ring near the AF interface would compensate the increase in magnetostatic energy by a decrease in anisotropy energy. We found that, for such configurations, operation is possible at much lower $|H_a|$ and considerably greater $M_s$.

The direction in which the DW departs the AF interface in an ideally symmetric MFNR and under a perfectly uniform applied field is arbitrary. The DW motion may be either in the clockwise (CW) or counterclockwise (CCW) direction during each revolution.
A preferred cyclicity can be established by biasing the applied field to more strongly affect one side of the ring across the AF interface than the other. Alternatively, a segment of the ring adjacent to a chosen side of the AF interface can be tapered, or made slightly softer, e.g., by ion irradiation [Chappert et al., 1998]. Similarly, exchange coupling to a soft composite element may be utilized [Suess et al., 2005]. It is also possible to design a system with alternating or configurable cyclicity by employing exchange biasing [Jung et al., 2005] and magnetostatic interactions with coupled or adjacent nanomagnets [Jain and Adeyeye, 2008]. The results in Fig. 13.6 were obtained for a nanoring with reduced anisotropy (10%) in a short segment immediately right to the AF interface, as illustrated in Fig. 13.7a. Consequently, the DW motion was in the CW direction during the simulation (Fig. 13.8).

We note that the fluctuations in the vertical magnetization component $m_z$ seen in Fig. 13.6 correspond to short intervals of backward motion of the DW during its advance forward. This phenomenon, known as Walker breakdown, is due to an instability of the DW structure under fields greater than the Walker threshold field, $H_{W}$.

The time required for the DW to complete a full revolution can be varied by changing the strength and periodicity of the applied field. Figure 13.8 shows the azimuthal

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure13.7.png}
\caption{(a) MFNR with an irradiated (low anisotropy) region (colored blue) adjacent to the AF interface (red); (b) MFNR magnetostatically coupled to a magnetically soft nearby nanomagnet (blue).}
\end{figure}
angle $\varphi$ (relating the DW position, Fig. 13.3a) versus time for six alternating applied fields ranging in strength from 100 Oe to 3 kOe, having the same rise and fall times ($\tau_a = 0.5$ ns) and frequencies of switching ($f_a = 0.0067$ GHz) as in Fig. 13.6. The upper-left inset shows that the DW mobility $dv_{DW}/dH_a$ is negative from 100 Oe to 300 Oe, and positive for $H_a > 300$ Oe. The two regimes correspond to the non-linear and linear precessional regimes, consistent with Walker theory [Mougin et al., 2007]. A linear steady regime, expected for $H_a < H_W$ is not seen here since for our system $H_W$ is low. Similarly, the bottom-right inset shows the time required for the DW to execute a full revolution for a given $H_a$. The frequency of revolution can therefore be tuned by adjusting the applied field intensity and period of switching. Modulating material and structural parameters can also serve to tailor DW mobility to access either the non-linear or linear precessional regime for a particular range of field amplitudes. Other recently proposed techniques for tuning DW mobility include the use of composites [Lee et al., 2007a], comb [Lewis et al., 2010] or wavy strips [Piao et al., 2009], spin-orbit interactions [Miron et al., 2011], and antiferromagnetic coupling (section 13.3).
The range of distinct operation frequencies can be advantageous for the performance of potential devices. The fact that the DW, upon reaching the AF interface, is stationary until the applied field is reversed implies that a strict synchronization of field periodicity with the period of DW revolution is not mandatory for operation, and that a margin of error is tunable by adjusting the field frequency. The flat energy landscapes and closed-path geometry make MFRNs convenient for studies of stochastic behavior and propagation paths at long time scales [Ravelosona, 2009], [Kläui et al., 2001]. In the case of MFRN spin-valves or tunnel junctions with currents perpendicular to the plane (CPP), the effects of spin polarized currents on DW dynamics can also be investigated [Burrowes et al., 2008]. MFRN spin-valves or MTJs (magnetic tunnel junctions) with CPP would be unique in that the high conductivity channel would be a function of DW position which itself would depend on the history of transmitted spin-current and applied magnetic fields. The cyclicity (digital) and DW position (analog) could be used as detectable logic outputs in potential magnetic circuits. For memory applications, MFRNs with energy landscapes containing wells at least $45k_B T$ deep could be used for long-term stability, where $k_B$ is the Boltzmann constant and $T = 300$ K. This implies the use of MFRNs with notches (Fig. 13.5c), or week coupling at the AF interface (Fig. 13.5a).

13.2.4 Conclusions

In summary, MFRNs possess several distinguishing features suggestive of their usefulness for potential DW-based applications. As a result of magnetic frustration, only one mobile DW with an associated DW energy exists in the MFRN, as opposed to zero DWs or an even number of DWs that result in non-frustrated rings. The DW in a MFRN is in permanent existence, can dwell anywhere along the ring, and can never escape or be annihilated by another DW. Another key feature is that the energy landscape can be made very flat with a proper choice of material and structural parameters. As a consequence, an alternating magnetic field with a very small magnitude can controllably drive the DW in consecutive circles around the ring. It was shown that a full range of operations are possible in a MFRN with low applied field magnitudes. It was also shown that MFRNs can be biased in order to set a specified cyclicity of DW motion to either CW or CCW. Energy landscapes with barriers and wells were demonstrated. The unique features of MFRNs can be found appealing for both logic and memory applications.
13.3 Domain Wall Motion in Antiferromagnetically Coupled Nanowires

The prospects of DW-based memory and logic devices are closely tied to the degree to which reliable and rapid DW motion in NWs can be achieved. In this section, we consider the characteristics of DW motion in NWs consisting of two antiferromagnetically coupled soft magnetic layers (Fig. 13.9). We show that in such systems Walker breakdown is substantially deferred, and that the maximum achievable DW velocity can be much greater than in conventional single-layer NWs. Many other characteristics of DW motion in antiferromagnetically coupled NWs are also shown to qualitatively differ from those pertaining to the single layer case. We take a look into the mechanisms responsible for the unique response, and discuss device implications.

13.3.1 Model Geometry

Two models are considered for purposes of comparison. The first model is a single-layer magnetic NW with a rectangular cross-section of dimensions 20 nm × 4 nm.
Figure 13.10: Model systems: (a) single-layer magnetically soft NW with a rectangular cross-section of dimensions 20 nm × 4 nm; (b) compound NW consisting of two magnetically soft layers antiferromagnetically exchange coupled through a thin interlayer. (Fig. 13.10a). The NW is modeled as perfectly soft so that the magnetic anisotropy is entirely due to magnetostatics. The preferred direction of magnetization is therefore along the principle NW direction. The second model is a compound NW consisting of two magnetically soft layers separated by a very thin nonmagnetic interlayer (Fig. 13.10b). The nonmagnetic interlayer serves to antiferromagnetically couple the two magnetic layers. The thickness of the nonmagnetic interlayer is 0.5 nm. The cross-sections of the two magnetic layers are 20 nm × 4 nm.

The length of the NW in each model is ∼ 2 μm. However, we have devised a gimmick to allow for the DW to teleport from one region of a NW to another. Teleportation serves to prevent the DW from exiting the structure, so that our observation of DW propagation is not limited by the finite dimensions of the NW model. The two teleportation sites for the single-layer NW are illustrated in Fig. 13.11. In both models, the teleportation sites were placed sufficiently far from the NW ends to prevent artifacts in DW motion due to magnetostatic interference from the far edges. For the teleportation scheme employed here, it is important that the tetrahedral finite element meshes in the two corresponding teleportation regions (in each model) are identical in order to achieve seamless teleportation (Fig. 13.11). It is also necessary to allow for bidirectional teleportation, as the DW may dynamically change its direction of propagation under applied fields and/or currents, and thus may need to teleport to and fro (e.g., during Walker breakdown).
13.3.2 Simulation Results

Figure 13.12 shows the DW velocity $v_{DW}$ versus applied magnetic field $H_a$ (along the nanowires axis) for a single-layer NW (saturation magnetization $M_s = 800 \text{ emu/cm}^3$, magnetocrystalline anisotropy energy density $K = 0$, exchange stiffness $A = 1.3 \text{ µerg/cm}$, and damping $\alpha = 0.02$) and for the AFC dual-layer NW for different values of the saturation magnetization of the top layer $M_s^{\text{top}}$ (remaining parameters for both layers are same as for the single-layer NW). From the black curve, the Walker threshold field for the single-layer NW is estimated to be $H_{W}^{\text{single}} \approx 50 \text{ Oe}$. The shape of the curve agrees well with that obtained from the one dimensional analytical model [Mougin et al., 2007], for which a steady-state linear regime is observed for $H_a < H_W$, following a nonlinear precessional regime for $H_a > H_W$ during which $v_{DW}$ decreases with increasing $H_a$. We note that a linear precessional regime, which is often observed subsequent to the nonlinear precessional regime, and which is due to the onset of vortex dynamics, is absent in our plot. This is due to the fact that our NW width is only 20 nm, and thus sets a high cost for vortex formation for the field range studied.

Examining the curves for the AFC case, we see that the behavior of the dual-layer NW is most similar to the single-layer case when the effective saturation magnetization $M_s^{\text{eff}} = M_s^{\text{bottom}} - M_s^{\text{top}}$ is closest to $M_s$ of the single-layer NW. As $M_s^{\text{eff}}$ is reduced
Figure 13.12: DW velocity $v_{DW}$ versus applied magnetic field $H_a$ (along the nanowires axis) for a single-layer NW (saturation magnetization $M_s = 800$ emu/cm$^3$, magnetocrystalline anisotropy energy density $K = 0$, exchange stiffness $A = 1.3$ µerg/cm, and damping $\alpha = 0.02$) and for AFC dual-layer NWs for different values of the saturation magnetization of the top layer $M_{s\text{top}}$ (remaining parameters for both layers are same as for the single-layer NW).

(i.e., as $M_{s\text{top}}$ approaches $M_{s\text{bottom}}$), the Walker breakdown field $H_W^{AFC}$ for the AFC case is pushed toward greater values, while the peak DW velocity $v_{DW}(H_W^{AFC})$ significantly increases. This is distinctly in contrast to the single-layer NW, where reducing $M_s$ lowers $H_W$ [Schryer and Walker, 1974].

Figure 13.13 shows the velocity dependence on the damping parameter $\alpha$ for the case of AFC NWs in the pre-Walker breakdown regime. Here, similarly as for the case of single-layer NW, reducing $\alpha$ increases DW mobility $dv_{DW}/dH_a$.

13.3.3 Physical Considerations

We first consider the case of the single-layer NW. Since the magnetic anisotropy is entirely due to magnetostatics, the magnetization of the NW lies along the nanowire axis everywhere in the structure, except in the vicinity of the DW, where a deviation from such alignment is occasioned by the transition in magnetization orientation. Figure
13.14 shows possible orientations of the central DW moment vector from the perspective normal to the NW cross-section. In Fig. 13.14a, the DW moment points along the axis corresponding to the larger of the two dimensions defining the rectangular cross-section. Therefore, this configuration is the least costly of the configurations in Fig. 13.14 in terms of magnetostatic energy. The effective magnetic charges due to the magnetization which have been added to the figure serve to illustrate this point. At zero applied field, the equilibrium state in Fig. 13.14a is the least costly configuration.

When a magnetic field is applied down the NW, the central DW moment experiences a precessional torque \( \tau_{\text{prec}}^a = -\frac{1}{1+\alpha^2}\hat{m} \times H_a \) (see (2.1)) which tilts it from its former equilibrium orientation toward a less magnetostatically desirable state (Fig. 13.14b). This tilting gives rise to effective magnetic charges and a demagnetization field in the \( z \)-direction, \( H_d \). The demagnetization field produces a precessional torque \( \tau_{\text{prec}}^d = -\frac{1}{1+\alpha^2}\hat{m} \times H_d \) on the DW moment which instigates DW propagation down the axial NW direction (\( x \)-direction). The damping torque (2.3) due to the applied field \( \tau_{\text{damp}}^a = -\frac{\gamma\alpha}{1+\alpha^2}\hat{m} \times \hat{m} \times H_a \) contributes to the propagation of the DW down the NW,
which can be understood by considering the extended DW profile. The damping torque due to the demagnetization field $\tau_{\text{damp}} = -\frac{2\alpha}{1+\alpha} \hat{m} \times \hat{m} \times H_d$, on the other hand, works to prevent the DW moment from tilting too much from the initial configuration shown in Fig. 13.14a. If the applied field is not too large, an equilibrium tilt angle $\theta_{\text{eq}}$ is achieved, and the DW steadily and rigidly propagates down the NW. While both $\tau_{\text{prec}}$ and $\tau_{\text{damp}}$ contribute to DW propagation as $\theta$ grows, it is the latter which is responsible for DW advancement once $\theta_{\text{eq}}$ has been reached. If the applied field, on the other hand, is increased beyond a critical point, the DW moment will undergo precession around the principle NW axis for as long as the magnetic field is applied. On the whole, the DW will advance forward. However, when the tilt angle passes from a region where $\tau_{\text{damp}}$ and $\tau_{\text{prec}}$ are equally oriented to a region where the two torques oppose (Fig. 13.15), the DW will slow down or move backwards. The phenomenon is known as Walker breakdown, and the critical applied field associated with its onset is called the Walker field. The intervals of the backward motion are due to the change in the energy gradients as the DW surmounts a magnetostatic energy peak. The torque $\tau_{\text{damp}}$ is responsible for the overall forward advancement of the DW wall, while $\tau_{\text{prec}}$ acts either as an acceleration or deceleration agent, depending on angle extended by the DW moment (Fig. 13.15). A complete model accounting for Walker breakdown can be found in [Schryer and Walker, 1974].

We now consider a DW pair in an AFC NW. Figure 13.16 shows possible configurations for the two central magnetic moments of the DW pair. The difference in
magnetostatic energy between the two configurations is greater for the case of an AFC NW than for the corresponding single-layer NW, as an extra magnetostatic energy penalty has to be paid to reach the state in Fig. 13.16c due to magnetostatic interlayer interactions. The encountered head-to-head (or tail-to-tail) configuration in Fig. 13.16c is magnetostatically less favorable than the head-to-tail configuration of Fig. 13.16a, owing to the finite lateral dimensions of the DW. Consequently, the damping torque contribution due to the demagnetization field, which opposes large tilt angles, is greater in an AFC NW than in the corresponding single-layer NW, and hence the Walker field is also greater.

It is known that in single-layer NWs, modulating $M_s$ and $\alpha$ only affects the Walker field $H_W$, and not the peak DW speed $v_{DW}(H_W)$. In order to understand the extent to which AFC systems defer Walker breakdown and to explain how peak DW speed of AFC NWs depends on $M_s$ (Fig. 13.12) and $\alpha$ (Fig. 13.13), it will be necessary to analyze the precessional and damping torque contributions of all fields involved while taking into account the DW structure rigorously. A detailed description of such an analysis is forthcoming.

### 3.3.4 Applications

AFC NWs offer a means of differing Walker breakdown and enhancing peak DW velocities. AFC NWs can thus be found attractive for envisioned DW-based applications, such as DW memories and logic. They may also serve as model systems to aid further

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**Figure 13.15:** Cross-sectional view showing the torques acting on the central DW magnetic moment vector for two representative tilt angles.
understanding of DW processes in composite systems, since a larger $H_W$ implies reduced sensitivity to interference from the neighborhood and from the thermal background. Lastly, the fact that an applied field tends to separate two DWs comprising a DW pair in an AFC NW, while a spin polarized current passed down the AFC NW would provide push on the two DWs in the same direction, suggests new operational possibilities and dynamical modes under field and current biases. For example, reducing the exchange coupling between the layers would allow DWs to wander from each other over some distance during propagation. This would imply dynamically changing Walker breakdown criteria, and could lead to intriguing DW dynamics thus far unobserved. Investigations of DW motion in AFC NWs with perpendicular magnetic anisotropy under field and current biases could be especially beneficial for future DW memory and logic devices.

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13.4 Crosswire Logic

13.4.1 Introduction

A logic is presented whose basic operational unit consists of two magnetic nanowires (NWs) running perpendicular to each other, with a small vertical offset to avoid contact at the crosspoint (CP). Networks of such units are considered at the end of the section. The networks could serve as model systems for the study of frustration effects and disorder dynamics. Connections are made to other physical systems.

13.4.2 Principles of Operation

The operation of crosswire logic relies on the magnetostatic interaction between mutually crossing NWs. Perpendicular magnetic anisotropy therefore is a prerequisite for such devices. Consider a uniformly magnetized NW overcrossing a second containing a domain wall (DW), and assume a downward oriented global magnetic field. The system is depicted schematically in Fig. 13.17a. The DW in the horizontal (with respect to the page) NW will be field-driven toward the CP. Once reaching the CP, the DW will cease to propagate if the magnetostatic field from the vertical NW is contrary to the applied field and of a greater magnitude. We shall always consider the strength of the applied field (or current, in case of current-driven DWs) to be inadequate to push the DW through the CP if the magnetostatic interaction opposes this dynamic.

Depending on how the described logical unit is interfaced with its surroundings, the sign of the applied field (or current), DW sense, DW position, and magnetization direction of the vertical NW could all be considered as logical inputs (Fig. 13.17f). DW sense here indicates whether the magnetization to the left of the DW is upward (positive sense) or downward oriented (negative sense). The logical output may now be defined to reflect whether the DW transited through the CP or halted. Consider, for example, a crosswire logic gate in which the DW sense represents the only logical input, and assume upward magnetization of the arbitrating vertical wire. Additionally, consider that the applied field is clocked for one full cycle, with the first half cycle corresponding to upward-oriented field, and the second half cycle corresponding to downward-oriented field. After one full cycle, the DW will be found right of the CP if the DW sense was positive, and left of the CP if the DW sense was negative. The logic unit hence serves as an IDENTIFY or NOT gate, depending on the relative designation of Boolean values (1 and
Figure 13.17: Crosswire logic unit: (a) two perpendicular magnetic anisotropy nanowires running perpendicular to each other with small vertical offset to avoid contact; (b)–(e) initial and final DW positions after half cycle of clocking field; (f) possible definitions of logical input and output values, with accompanying truth tables for several Boolean operations.
Figure 13.18: Concatenation of crosswire logic units showing initial and final DW positions after two and a half clocking cycles. The magnetization of vertically running nanowires arbitrates DW propagation.

0) of the logical input and output states, and depending on the phase of the clocking field. Were the sign of the applied field to constitute the second logical input, the described unit would operate as a XOR or NXOR gate. Alternatively, if the magnetization orientation of the vertical arbitrating wire were to be considered as a second input, AND, NAND, OR, and NOR gates could be realized as well (see Fig. 13.17f for examples.) The question now is how are input states received or prepared, and how can multiple logic gates be cascaded to form larger circuits.

13.4.3 Concatenability

Consider a system of one horizontal NW and a series of equispaced vertical arbitrating wires. Here, the magnetization directions of the vertical wires together with the initial state of the DW are considered as logical input, and we assume a global clocking field. The described system can be viewed as a concatenation of logic units where the output of one unit (gate) serves as input to the next. As shown in Fig. 13.18, the input values determine where the DW is to be found after a given number of clocking cycles. Once the DW passes an arbitrating wire, it cannot cross back if the magnetization of the arbitrating wire remains constant.

By allowing for vertical DW transit, the magnetization of the arbitrating vertical wires can be manipulated as well. If the thickness of the vertical wires exceeds that of the horizontal wires, or if the saturation magnetization of the former is greater, the horizontal wires will not affect the configuring of the vertical wires. However, if all wires are identical, mutual arbitration is realized. Mutual arbitration of DW motion between
the vertical and horizontal NWs together with the bidirectionality of DW propagation under a clocking field suggest the possibility of iterative-like operation where an operand may return to be processed multiple times by the same physical unit(s) under variable configurational settings before it is finalized for output (cf. Fig. 13.18). This implies the possibility of architecture reuse or multilevel processing on single level logic circuitry, unique to the CW paradigm.

13.4.4 Connection to other Physical Systems

Mutual arbitration and bidirectionality impart properties to crosswire architecture which make it analogous to other physical systems. Consider a two-dimensional crosswire matrix with some arbitrary DW configuration as may be obtained subsequent to magnetization relaxation following in-plane saturation (Fig. 13.19a). Application of a periodically oscillating perpendicular magnetic field will result in the movement of DWs, the mobilities of which at each field cycle are subject to CP arbitration that reflects the instantaneous magnetization configuration of crossed NWs. While CP arbitration checks the transit of DWs across CPs, the DW configuration ensuing after each field cycle modifies subsequent arbitration. The question becomes, does the DW configuration ultimately converge. In

Figure 13.19: Drawing a parallel between (a) a crosswire network and (b) a spin ice system.
spin ice systems, such as the kagome lattice in Fig. 13.19b, magnetic frustration effects lead to a highly degenerate ground state (GS) [Rougemaille et al., 2011]. Frustration also affects how the system journeys from a highly frustrated higher energy state to one of the less frustrated GSs. A further connection can be made to magnetization relaxation of a magnetic system under non-equilibrium conditions. Consider an ensemble of spins coupled to a zero temperature thermal background, and assume some level of disorder was instantaneously introduced to the spin system. The spins will eventually coalign and orient along the preferred direction, thus achieving uniform magnetization, and reaching the GS. However, the greater the level of disorder initially introduced, the longer the journey will be to the GS [Kazantseva et al., 2008], as the gross disorientedness of each spin and its neighbors does not provide immediate clue to the final state. Crosswire architecture, therefore, may also serve as a model system for the study of frustration effects, disorder dynamics, entropy, and pathways to the GS. The relevant GS need not necessarily be the energy GS, but a configurational or logical GS. Crosswire systems could thus reveal routes toward new algorithms and non-standard circuits for future applications.
Bibliography


