SPIN-VALVE INTERFACE FOR MAGNETIC QUANTUM DOT CELLULAR AUTOMATA

A Thesis

Submitted to the Graduate School of the University of Notre Dame in Partial Fulfillment of the Requirements for the Degree of Master of Science in Computer Science and Engineering

by

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April 2008
CMOS technology is reaching its physical limits in terms of scaling, and this is leading many researchers to investigate alternative computing technologies. As the industry moves away from CMOS and toward other technologies, it will be necessary to explore new ways of transporting data. This thesis explores a novel application of two relatively new technologies, magnetic quantum dot cellular automata and spin-valve technology, with a focus on existing work in magnetic random access memory. To move forward in the real-life implementation of new computing technologies, some new engineering will be necessary to bridge the gap between extant CMOS computing technology and this new area of magnetic logic and storage. With a view toward promoting this, the spin-valve-based Magnetic-Electric Interface (MEI) was developed. Topics covered in this thesis include the state of the art of the technology behind MQCA as well as the reasons for using it, spin-valve technology such as MRAM, the reasons for development of, rationale for and design behind the MEI, and potential applications of the technology for development of MQCA computing systems.
To my mother, who instilled in me a love of reading and writing, and to my father, who instilled in me a fascination with math and science.
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ACKNOWLEDGMENTS

First, I would like to thank and acknowledge my advisors, Dr. X. Sharon Hu and Dr. Michael T. Niemier, for their advice and support during “the grad school process.” They have both performed expertly in helping me shape my mind around the process of research and helping me “learn how to learn.”

Thanks also to my research group, especially A.J. Dingler and Michael Putney, both of whom have variously assisted me a great deal with debugging code, analyzing results and general sounding board duty.

I am very grateful to the “MuMag” OOMMF development and user community at NIST, especially Drs. Michael Donahue and Donald Porter, who have provided me with both a top-quality simulation package to work with and a great deal of technical support for said software package.

Special thanks to Timothy Brick and Philip Little of the Computer Science and Engineering Department both for their invaluable assistance with coursework and their friendship.

Finally, thanks to the Schmitt Fellowship here at Notre Dame, not only for their funding but also for their inspiration.
CHAPTER 1

INTRODUCTION

It is generally accepted in the integrated circuits industry that within the next fifteen to twenty years, methods for improving scaling down in CMOS transistors will encounter a number of roadblocks due to device-level physics limitations such as electron tunneling and the limits of photolithography. As the ability to scale down CMOS decelerates, engineers will necessarily need to search for replacement technologies that are capable of maintaining the downward trends of feature size while retaining the ability to be used in a variety of applications in order to improve performance.

A number of potential device-level and architecture-level solutions for this problem have been explored, such as nanowire logic (Huang et al. (2001)), FinFETs (Nowak et al. (2004)), CMOS-molecular hybrids (CMOL) (Strukov (2005)) , field-programmable nanowire interconnect (FPNI) (Snider (2007)), and various implementations of quantum dot cellular automata (QCA). This thesis will focus on one particular type of QCA, magnetic QCA (MQCA), which makes use of single-domain nanomagnets (at about the scale of 60 nm by 90 nm) aligned with each other in series to both perform calculations and function as “wires” which transmit data from one region to the next.

There are a number of reasons to examine MQCA as a replacement technology for CMOS. First, no electric current flows through MQCA devices; rather, they use
orientations of magnetic domains in nanomagnets to represent logic states. This means that they can dissipate very little power during computation compared to CMOS. Second, the fact that the technology uses the same elements for both wires and logic means that the VLSI designer’s job is significantly easier in a computational sense; interconnect is becoming more and more of a problem in CMOS-based circuits just as logic is, and since data moves in a systolic way through devices, nothing is “lost” by using MQCA wires as interconnect. Finally, scaling MQCA down is much easier than in CMOS, creating the potential for much greater logic (and wire!) densities.

This thesis describes a device, the magnetic-electric interface (hereafter abbreviated as “MEI”) based on spin-valve technology which can be used to “read” nanoscale MQCA data out into a CMOS device. It will discuss the rationale and development in simulation of this device, potential methods for fabrication, and possible uses for the technology in the future.

1.1 Existing Work in MQCA and Spin-Valves

The QCA system designer can approach MQCA knowing that the technology has already been extensively studied and that there exist multiple examples of working devices (Imre et al. (2006b)), including majority logic gates, wires, and tools for input. Power studies have also been conducted (Alam et al. (2007)) and compare quite favorably to CMOS. Thus, MQCA seems to be a promising avenue for further exploration.

The spin-valve device, based on the giant magnetoresistive (GMR) or tunneling magnetoresistive (TMR) effect, was first characterized in 1986 (Baibich et al. (1988)). It permitted sweeping changes and enhancements to magnetic data stor-
age technology, and soon hard drive read heads based on the technology were developed. Today, the technology is used in hard drives, magnetic RAM, and micromagnetic sensors, among other places.

1.2 New Research in Magnetic-Electric Interfaces

We have combined research in MQCA with research in spin-valve devices to create the MEI, which uses the magnetic flux in MQCA devices to set the magnetization state of the spin-valve. There were a number of hurdles to overcome – interference within the device from one magnetic layer to another, managing timing between the MQCA and MEI, and dealing with increased power required to allow the MEI to function compared to the MQCA elements.

After addressing these concerns, we have developed a design which has been shown to work well in a variety of environments and a reasonable tolerance for manufacturing error. We have explored the design and construction of this device, as well as the testing methodology and rationale behind its development. We have also investigated the results found in simulation and what they mean for manufacturability as well as error tolerance. Finally, we will discuss in this document potential applications for this interface device, including MQCA system output to CMOS and the potential for bridging signals from one part of an MQCA device to another.

1.3 Organization

The rest of this thesis is organized as follows:

- Chapter 2 discusses existing work in related fields and discusses some basic background information.
• Chapter 3 features the theory behind the operation of the MEI and includes some information about the basic design.

• Chapter 4 provides simulation details and results of testing.

• Chapter 5 concludes and speculates on future work in this field.
CHAPTER 2

BACKGROUND AND RELATED WORK

This chapter reviews the current state of the art as well as the history of development of the set of technologies on which the MQCA-CMOS interface depends. Among these are QCA technology in general and magnetic QCA in particular (originally developed by researchers at the University of Notre Dame (Csaba and Porod (2002))), giant magnetoresistive magnetic hard drive read head technology, originally developed (and now licensed) by IBM, and tunneling magnetoresistive technology (which makes MRAM possible).

2.1 QCA Basics

It helps to understand why we study magnetic QCA if we take a brief look at the other QCA technologies. The two types currently studied are electrostatic, which has a number of “subset” technologies, and magnetic, the subject of this thesis.

2.1.1 Electrostatic QCA

The three implementations of electrostatic QCA, metal-dot, semiconductor, and molecular, all share basic elements of functionality. They consist of an array of four or six quantum dots laid out in an equidistant pattern, forming a QCA
“cell.” Opposite charges in the form of two electrons “caught” in the array of quantum dots are assigned to two neighboring corners of a cell, which then force the electrons in that cell into an orientation opposite the charges. The system designer arbitrarily chooses one orientation of charges to represent a logical “0,” and the other to represent a logical “1.” In the case of six-dot QCA cells, the electrons sit in a lower energy state in the two dots in the middle of the cell, awaiting the application of the clocking field to excite them into the correct logical state. This effect “dominoes” down the adjacent cells as shown in Figure 2.1 due to nearest-neighbor interactions between the cells. The clocking field is moved in one direction across the cells in a repetitive fashion known as a “computational wave.” This technology has been described by other researchers at the University of Notre Dame in the past (Lent et al. (2006)). In this way data moves systolically down a “wire” of QCA cells.

To perform logic calculations, cells are arranged in a “cross” pattern as shown in Figure 2.2. The north, west, and south cells are polarized by their neighbors,
Figure 2.2. Diagram of an electrical QCA majority gate structure. It is worth noting that majority gates in MQCA function in much the same way.

and the center cell polarizes according to the majority of the inputs. The resulting logical value is then propagated out of this majority gate by the east cell. Inversion is possible thanks to structures like the one also shown in Figure 2.1. With these three structures, a complete combinational logic set is available to the QCA system designer.

Metal-dot QCA is attractive largely owing to the fact that its functioning has been repeatedly experimentally demonstrated (Tougaw and Lent (1993)). With operating temperatures around 15mK (Orlov et al. (1997)), however, it is impractical for most applications. The related semiconductor QCA is useful largely for prototyping, as current CMOS processes do not lend themselves to mass-production of devices.
Molecular QCA would be a very promising technology, given that it features operation at room temperature, extremely small feature sizes (cells on the order of 1nm on a side), and the potential for self-assembly \cite{Sarveswaran et al. (2003)}, were it not for large defect rates that currently make useful device fabrication infeasible.

2.1.2 Magnetic QCA

Magnetic QCA leverages structures similar to those found in electrostatic QCA—majority gates and wires consisting of cells connected in series. Rather than representing logical states as arrangements of charge, magnetic QCA represents them using orientations of magnetic domains in nanomagnet structures on the scale of 60 nm x 90 nm. An electrical input structure can be used to set the initial magnetization of the first MQCA element in a series of cells. The MQCA system designer arbitrarily chooses one orientation, “down,” for example, to represent logical “0” and the other as logical “1,” similar to the logical paradigm found in electronic QCA. An external magnetic clocking field is then applied to the MQCA cells in the direction of the hard axis of the magnet, causing its magnetization to rotate into a logically indeterminate state between “up” and “down.” When the clocking field is relaxed, the MQCA cells begin to settle into either an “up” or “down” state based on the state of the cells next to them. This can be seen in Figure 2.3, which illustrates the process in a simple diagram.

Materials for constructing these nanomagnets should meet a number of criteria \cite{Imre (2005)} for optimum performance. First, they should possess low coercivity, which is defined as the strength of the magnetic field required to reduce a material’s net magnetization to zero after having been brought to saturation by
Figure 2.3. Diagram showing the progress of MQCA elements changing their magnetization in response to a change in input and application of a clocking field.
another field. This is important because speed of switching and low field strength for switching are both highly desirable in MQCA components. Lower coercivity means a lower-strength clocking field is usable for clocking the MQCA elements. It also enables the field to be switched on for a shorter length of time. The magnets should also have strong anisotropy: a tendency to magnetize in one direction or another. The easiest way to accomplish this is via so-called shape anisotropy. This is the often-observed tendency (in bar magnets, for example) for magnets to align their magnetization along the longest axis of the magnet. The goal of manipulating shape anisotropy in an MQCA magnet is to cause its magnetization to tend to orient strongly in one of two directions along its easy axis, thus producing a measurable, bistable state for the magnet when performing logic. When the clocking field in an MQCA system is relaxed, the cells settle “up” or “down” due to the shape anisotropy resulting in these being the lowest energy states of the magnetization. Finally, it is desirable for the material chosen to have a remanent magnetization equal to its saturation magnetization; that is, no magnetization should be “lost” when the clocking field is switched off. This ensures that the magnets retain the ability to propagate the correct polarization from one cell to the next in the absence of the clocking field.

Figure 2.4 illustrates a typical nanomagnet in the OOMMF micromagnetic simulator and the process of switching its state from “0” to “1.” As a value progresses down an MQCA wire, it inverts from one cell to the next. This feature, combined with the majority gate, produces a complete combinational logic set. All of these MQCA devices have been experimentally confirmed to work in real, fabricated material, with the caveat that they were operated under carefully controlled, somewhat practically unrealistic conditions.
For example, Imre’s MQCA wires and majority gates were operated with clocking field strengths of 200-500mT, and the fields were relaxed over a time period of about 30 seconds on average. Desired switching times for logic states in MQCA devices are on the order of nanoseconds, and desired field strengths in the tens of milliTesla at the most. Nevertheless, these experimental data confirm the principles at work to be valid, and we can be reasonably confident that the specifics in terms of time and field strength are largely a matter of trial-and-error engineering to narrow down.

Imre needed to use strong fields and slow clock field relaxation times for good reason: the wires under consideration simply would not polarize correctly without them. Without something — a block of magnetic material with its magnetization pointing in the direction of the MQCA’s hard axes, or an applied magnetic field in the same direction — “holding” the output end of the wire and preventing it from settling, the pattern observed in any long wire produces a logically wrong result. The output end becomes prone to settling before the middle of the wire settles and sets it to the correct value.

We have previously mentioned in this chapter the “computational wave” clocking field proposed for use in EQCA. A similar clocking paradigm can be used in MQCA (Alam et al. [2007]). This phased clocking scheme gives rise to the potential for certain kinds of deeply pipelined applications to be particularly applicable to QCA architectures. We can make use of the MEI to perform a kind of “fast forwarding” through the pipeline, as we will discuss later.

There are a number of other features of MQCA that make it particularly attractive to study with a view towards implementing real systems in the near-term future. First, MQCA consumes relatively small amounts of power (Alam}
Figure 2.4. Simulation output from the OOMMF micromagnetic simulator. The beginning of a transition from one state to the other is visible as a significant change in overall magnetization from “up” to “down,” starting at the top where the magnetization is being “bent” to the right (and eventually down) by an applied magnetic field.

Second, it is impervious to the effects of radiation such as radio interference or cosmic rays. This makes it a natural choice for systems which must function at their normal speeds in radiologically harsh environments such as space. Third, it functions well in a wide range of temperatures, including room temperature. Finally, it is fairly easy to fabricate (if not mass-produce) working devices such as wires with current technology. This has already been demonstrated in several examples of previous work (Imre (2005)).

There are, of course, some problems with doing MQCA system design; one of these is the question of performing input and output to and from CMOS. CMOS input to an MQCA device is largely a solved problem. Using the same technologies proposed for clocking large regions of MQCA cells, we can “clock” a single cell with a clocking field oriented in a direction orthogonal to the rest of the clock zones on the chip. In this way, we produce a biasing field from the input cell to the other MQCA cells which directs the MQCA devices in the desired orientation as shown in Figure 2.5. This method should work well based on previous real-world studies.
Figure 2.5. Prospective design for an MQCA input based on existing MQCA clocking structures.

involving similar structures (Imre (2005)).

Output, however, is a much more complicated problem. Currently the method for ascertaining the value of any given cell is to simply image the entire chip with a magnetic force microscope. While this produces quite thorough results (Imre (2005)), it is impractical for production work. There does exist some precedent for reading the orientation of extremely small magnetic fields both in the computer hard drive industry (Tsang et al. (1998)) and in the magnetic RAM industry (Andre et al. (2005)) with the use of spin-valve-type structures. The question then becomes, what scheme shall we use to utilize this type of solution in the most reliable way? We will discuss this subject in Chapter 3.

2.2 Magnetic Spin Devices

As the MEI is spin-valve device, it is important to discuss the background of these before delving into the design of the MEI. In Chapter 3, we will discuss how
the MEI shares some similarities with GMR hard drive technology and some with MRAM technology, but is different from both in several key ways.

2.2.1 Giant Magnetoresistance

Devices based on nanomagnetism have a rich, if relatively recent, history. Since the 1990s, organizations such as IBM have been conducting research into applications of the GMR (giant magnetoresistive) and related TMR (tunneling magnetoresistance) effect. The most widely used of these are in magnetic hard drive read heads, which use the change in resistance created by a free-layer magnetic orientation change to read the data stored on a spinning drive platter (Belleson and Grochowski (1998)).

The GMR effect was discovered in 1988 (Baibich et al. (1988)), almost by accident, by researchers studying the applications of metallic multilayers of magnetic and nonmagnetic materials. It was described as ”giant” magnetoresistance because the change in magnetoresistance displayed in the materials used was so much greater than the magnetoresistive effects that had been studied until then – primarily anisotropic magnetoresistance, the property of some materials to change their electrical resistance simply in the presence of a magnetic field. The GMR technology was quickly refined, and by 1997, IBM had released a commercial hard drive product using read/write heads that took advantage of the effect.

The best analogy to describe how giant magnetoresistance works might be the example of light passing through a pair of polarizing filters. With one filter, the light passing through is reduced by some percentage. With two filters, the light passing through may be reduced by 100% or, in fact, by the same percentage as with only one filter, depending on how the second filter is rotated. If its
polarization matches the polarization of the first filter, no additional change in light transmittance is seen. If its polarization is exactly orthogonal to that of the first filter, the amount of light passing through the two filters is reduced to zero (or near-zero).

The giant magnetoresistive effect functions in a similar fashion. Instead of polarizing filters, GMR occurs between layers of magnetized metal with a non-magnetic, conductive spacer between them. In addition to voltage, electric current has the property of “spin,” the angular momentum of the electrons flowing in it. When current passes through a layer of magnetized metal, some of it becomes “spin-polarized” as shown in Figure 2.6. At the points where there exist metal boundaries in the GMR multilayer, the electrons experience a scattering effect, increasing the resistance experienced by the current passing through the device. When the two (in this case) layers of magnetic material have parallel magnetizations, the scattering is minimized, but when their magnetizations are antiparallel (along precisely opposite angles), there exists more scattering, and the magnetoresistance experienced in the device increases. In some experimental multilayers, this magnetoresistance change can be as much as 50% (Baibich et al. 1988). Typical delta in most extant magnetoresistive devices, however, is closer to 12-25%. Magnetoresistive devices that function in this way are referred to as “spin-valves” because they let varying amounts of electric current through them dependent on the current’s spin.

2.2.2 Tunneling Magnetoresistance and MRAM

A related effect also used in existing products on the commodity market is the tunneling magnetoresistive effect (TMR). The principle at work is nearly the same,
with the exception that rather than a conductive spacer sandwiched between two magnetic layers, TMR devices possess a thin, resistive, tunneling barrier layer between two magnetic layers. The current spin-polarizes in the same manner as in GMR devices, and as in GMR devices, this effect is the source of the change in magnetoresistance. Current tunnels across the thin (about 1nm) barrier, and the magnetoresistance changes depending on the relative orientation of the magnetic layers. An example implementation of this effect is seen in the comparison diagram shown in Figure 2.7, which describes the general layout in cross-section of Freescale’s commodity MRAM part.

Freescale’s MRAM device is an example of an existing application of the TMR effect. A single TMR MRAM cell as implemented by Freescale is a fairly simple structure, with layers of metal and oxide similar to the magnetic-electric interface (MEI) we will describe in Chapter 3. Additional hardware is necessary, however, to take an orientation of toggled free layers and write to it in such a way as to
Figure 2.7. Diagram illustrating in cross-section the existing Freescale TMR MRAM construction. Diagram courtesy of Freescale, Inc.
store a value for later retrieval and produce a result when queried in terms of a logical “1” or “0.”

To write a bit to an element of MRAM, it is necessary to expose it to a magnetic field of sufficient strength. If all one were concerned with was a single bit on a chip, this would be a trivial affair: simply expose the MRAM cell to a field oriented in the vector of choice, and the (single) free layer in the cell would change magnetization to match it. The fixed layers in the cell would not be affected (or be affected very little at first, and ultimately not at all), since the bottom layer would be pinned by the attached antiferromagnetic layer, and the upper fixed layer would be strongly encouraged to stay antiparallel to the bottom thanks to its close proximity. This approach obviously becomes problematic when one wishes to have an array of MRAM bits on the same chip in close proximity to each other; how does one choose which cell to write? Putting them in a line would simply change all of them at once. Figure 2.8 shows a simple circuit diagram of how MRAM is typically assembled, and how current flows through the device.

To solve this problem, Freescale made a number of changes to the construction of the MRAM unit. To begin, the free layer was turned into two free layers separated by a thin conductive spacer (much like the construction of the fixed layers). This produced a free layer system which could rotate freely in response to applied magnetic fields but was always in an antiparallel state like the fixed layers.

It is important to note here how the GMR/TMR effect could continue to work in a device constructed in this way. What is truly important to the state of magnetoresistance in a GMR or TMR device is the number of magnetization transitions in the device as current passes through it. In one case, where the free
Figure 2.8. Circuit diagram of MRAM device (Freescale [2007]).
layers are in the same orientation as the fixed layers so that the total system is in a “up, down, up, down” alignment (from bottom to top), the resistance is high, because there are 4 magnetization transitions for the current which moves through the device. In the “up, down, down, up” case, the resistance is lower, because there are only 3 transitions.

The free layers of the MRAM were not the only part of it that was changed; the writing mechanism was also affected. Since now there would exist no change in state in the device if a single magnetic field was applied to the device, two write lines, referred to as the “bit line” and “digit line,” were added to the design. The two lines apply a pair of magnetic fields, one after the other in series. The fields are carefully balanced and timed such that the magnetizations in the free layers “toggle,” (Andre et al. (2005)) i.e. each layer flips such that its vector points in the opposite direction regardless of what it was originally. This arrangement also solves an intrinsic addressing problem with MRAM in that both lines are required to activate in order to get the bit to flip. Activating only one line actually makes the bit more resistant to flipping. This avoids the “half-select” problem intrinsic to older, non-toggle style MRAMs.

This toggling scheme requires that precautions be taken in the operation of a working MRAM part. Before writing any arbitrary bit to an element of MRAM, the device must first test the bit to examine what value it currently contains. If the value is the same as the one the device wishes to write, no action is taken; otherwise, the bit and digit lines are activated and the value is flipped. This step is necessary because there is no way to simply “write a 1” or “write a 0.” The only action possible is to toggle the bit.

For reading, a set of electronics is necessary to analyze the resistance of the
MRAM bit and compare it to a pair of reference bits which are part of the device; that is, there are two bits of MRAM which are not designed to switch at all, but instead are included only for comparison to any given bit being read. One is fixed at ideal “0” and the other at ideal “1,” and the resistance of the MRAM bit is compared to these to determine what logic value it holds.

The Freescale design is substantially larger in area than the MEI at a micron on a side in its largest dimension, but we do not anticipate this to be a significant problem; existing GMR experimental devices of about the size of the MEI work well (Pohm et al. (1996)). The primary reason it is as large as it is is largely an issue of convenience for fabrication. Since flash EEPROM is remarkably inexpensive and suits most requirements for non-volatile solid-state storage, Freescale has been reluctant to use their “first-class” fabrication facilities to manufacture their MRAM parts, instead devoting them to other devices. Because of this, current MRAM devices are fabricated on a 180nm process on older fabrication systems (Freescale (2007)). We note that the large area of the MRAM device contributes to its large resistance, but barely at all to its MR ratio (the difference between parallel and antiparallel states).

Our MEI design is very like the Freescale MRAM design, with the following exceptions:

- We have included only one free layer rather than the antiparallel twin free layers.

- We use no tunneling barrier but instead a conductive spacer between the fixed and free layers.

- The overall area of the device is much smaller.
We discuss the design of the MEI in more detail in Chapter 3.

2.3 Spin-Torque MRAM

It is worth a brief discussion of a particular type of MRAM known as spin-torque MRAM \cite{Ozatay2006} because the technology may potentially be useful as an MQCA input method. While we know existing clocking systems can be modified somewhat as input devices, the spin-torque method is somewhat more elegant. It involves a structure very like a combination GMR-TMR device, with a conductive spacer above the tunnel barrier. Part of the conductive spacer extends down into the tunnel barrier and directly touches the uppermost fixed layer of the device. When current passes through the device, it is spin-polarized (much as it is spin-polarized through a magnetic tunnel junction in an MRAM) and causes its free layer to magnetize in one direction or another. This occurs because the angular momentum from the spin of the “injected” electrons is transferred partially to the magnetic material.

This is notable as a possible MQCA input device primarily because of its improved flexibility compared to the “private clock zone” method we discussed earlier. The clock zone method requires that a certain (fairly large) amount of area be devoted to the input device, whereas with the spin-torque method all that is required is the structure itself and a metal via to carry current to it. The example found in the literature was 150x200nm, but this is hardly a problem, as larger magnets have larger fields which are more likely to bias the neighboring cells in the correct direction. This method of input has not been evaluated in simulation yet, but we have had repeated successes in earlier experiments in simulation involving larger magnets driving much smaller magnets – specifically, devices as large as the
1-micron Freescale MRAM driving 60x90nm MQCA elements.
This chapter presents proposed designs for tackling technical challenges in the development of a magnetic-electric interface (MEI) for nanomagnetic devices, which converts magnetic computing signals into electronic signals. The rationale behind the MEI design will be discussed, as well as some “lessons learned” during development and potential applications for a device of this type. We discuss the application of spin-valve technology to the MEI’s design, as well as present a discussion of necessary physical parameters for fabrication. We also present some insight as to how the design as discussed here might be constructed now as well as in the future.

3.1 Design Rationale

We have chosen a spin-valve design for the interface. A spin-valve, as noted in Chapter 2, is a device which takes advantage of one or more types of magnetoresistance to produce varying resistances in the device depending on the orientation of two or more layers of magnetic material within it.

Figure 3.1 illustrates the design of the spin-valve-based Freescale MRAM stack and how it compares to the antiferromagnetic stack we have chosen for the MQCA interface. The general idea of the interface is that the MQCA element adjacent
to the magnetic stack will exert a net force on the “free” layer of the spin valve such that the resistance through the device (i.e. if one were to pass a current through its z-axis) changes when the magnetizations of the layers are either parallel or antiparallel. This achieves the goal of converting magnetic logic signals into electrical logic signals which can be processed by CMOS technology.

Note that several constraints must be met here. First, the device must be robust to the imposition of strong magnetic fields, as they are part of the operation of any MQCA device during the phase when its clocking field is active. We have learned from the experience of Freescale, which has produced a commodity MRAM
part, in the construction of the pair of fixed layers which provide a magnetic “reference point” for the free layer. Second, the device’s free layer must be more free to change alignment than that of a comparably-sized, comparably-composed MRAM cell. In the case of writing to MRAM, one or more strong magnetic fields are used to write directly to the cell, and are localized to that cell. Enough magnetic force is applied to the cell to get it to flip in the direction of the force. This is not possible with the MQCA interface, which instead must allow its free layer to orient entirely along its hard axis and then be biased by the comparatively weak interaction with its neighbor MQCA cell. Third, the device must avoid undesirable interaction (known as “exchange”) between the free layer and its lower neighbor, the uppermost fixed layer, or it will always face a problem with the free layer biasing in whatever direction is opposite its lower neighbor rather than its adjacent neighbor.

3.1.1 Problems with Existing MRAM Devices

The essential idea behind the CMOS-MQCA interface was to take advantage of existing designs for MRAM and use them directly in an MQCA system. This presented several problems:

- The scale of existing MRAM systems is not commensurate with the scale of the MQCA devices we anticipate to be implemented.
- The switching mechanism of MRAM systems is wholly different from how one needs to switch an MQCA device.
- There existed some question as to how a suitable multilayer structure could be constructed, both with existing and theorized future technologies.
There was also some concern that the magnetoresistive effect (whether TMR, tunneling magnetoresistance, or GMR, giant magnetoresistance) would not change the resistance of the MEI device sufficiently to be detected by the matching circuitry which compares the device’s resistance to the two reference bits used to determine what its logical state is (Andre et al. (2005)). In part, this is because the magnitude of change in magnetoresistance is partially determined by the area of the device. Compare the scale of the extant Freescale MRAM part, about a micron on a side – with that of the typical MQCA cell, which is about 60 nm by 90nm in most current work. The MRAM part, which uses the TMR effect, gets a change in MR of about 12-15%, depending on operating conditions. This range is well within the tolerances of the matching hardware. Older, smaller experimental GMR MRAM devices (Pohm et al. (1996)) close to the scale of the MEI – about 200nm wide, in this case – also display a 12-15% change in MR. The change in magnetoresistance is also dependent on how thick the separation is.

3.1.2 Problems with Other Alternatives

A device based on a magnetic hard drive read head would seem to be a natural choice for reading MQCA data. The principle is essentially the same, but mechanically, of course, much simpler – all that would be required would be to position the tip of the read head directly over a cell to be read, and simply leave it there. One could fix it in place and it would function just as it does in a hard drive – changing resistance according to the magnetization of the MQCA cell below it rather than the data elements in the drive – but there is an important problem with this approach.

In terms of physical construction and mass-producibility, it is far from ideal.
TABLE 3.1

Comparison of Existing Magnetoresistive Technology

<table>
<thead>
<tr>
<th>Technology</th>
<th>Device Area</th>
<th>Separation</th>
<th>Delta-MR</th>
</tr>
</thead>
<tbody>
<tr>
<td>MEI</td>
<td>60x90nm</td>
<td>5nm</td>
<td>5%</td>
</tr>
<tr>
<td>IBM GMR HDD Head</td>
<td>200x100nm</td>
<td>1.5nm</td>
<td>12-15%</td>
</tr>
<tr>
<td>Early GMR MRAM</td>
<td>270x220nm</td>
<td>16nm</td>
<td>12-15%</td>
</tr>
<tr>
<td>Freescale MRAM</td>
<td>1000x850nm</td>
<td>1.1nm</td>
<td>12-15%</td>
</tr>
</tbody>
</table>

It is, in fact, not far away from simply using an MFM to image the chip, with the exception that it is not required to move. In both cases, the system designer needs to apply some additional piece of equipment to the MQCA chip. In the case of adding this theoretical hard drive read head, it must be done with utmost physical precision in order to be accurate and useful. Part of the goal of the MEI is to produce an interface device which can be constructed in lithography, as part of the rest of the chip. This saves complexity and enables more potential for mass-production.

We know from some previous work (Hempel (2005)) which investigated the magnetoresistive performance of various magnetic multilayer configurations that it is possible to obtain about 5% delta-MR with separation between free and fixed layers (conductive spacer thickness) of 5nm. Table 3.1 compares and contrasts some existing technology in terms of what change in magnetoresistance (labeled “Delta-MR”) can be expected from different area devices with different separations between free layers (labeled “Separation”) and fixed layers.
Recall that the general design of GMR devices includes a magnetically fixed layer, a conductive spacer (usually copper), and a magnetically free layer, the magnetization of which can be switched independently of the fixed layers below it. In an MRAM device, this is accomplished by some direct magnetization scheme; for example, the Freescale “toggle” scheme (Andre et al. (2005)) which uses two electrical “writing” lines to impose magnetic fields on the free layers of MRAM cells to “flip” them in one direction or another. With magnetic QCA, this approach is inapplicable, as the Freescale toggle method is, first, only for writing data, and second, only useful for toggled free layers which would be useless for MQCA interfaces.

Instead, we aim to “null” (that is, push the magnetization vector as much in the direction of its hard axis as possible) both the QCA devices and free layer of the MEI such that the next state of each cell – and of the MEI – may flip to the correct logic state determined by the previous set of MQCA circuitry. There exists a fundamental difference between MRAM and the MEI in the mechanism by which the free layer’s orientation is decided. In MRAM, the free layer’s magnetization is set directly by magnetic fields imposed upon it. By contrast, the MEI’s mechanism must be much more delicate. The magnetic orientation of the MEI’s free layer is nulled to point in the direction of its hard axis, and is then biased in a direction by its neighbor MQCA cell and allowed to relax in that direction. (See Figure 2.3).

The key difference between MRAM switching and MEI switching, then, is the source of the change, and mechanistic differences between those sources. MRAM devices can afford a certain degree of undesirable interaction between the free layers and fixed layers, because their magnetizations are being changed by external fields being applied directly to their free layers. The MEI, on the other hand,
depends on a comparatively weak influence from a neighboring MQCA cell to determine which orientation it should take.

It is important to note why we chose a device based on the conductive GMR approach rather than the electron-tunneling TMR approach, which is already in use successfully in existing MRAM parts. As we studied the problem of building a CMOS-MQCA interface, it was discovered that no matter how the device was constructed – the thickness of the layers, their metallic composition, the shape of the MQCA elements or the shape of the layers themselves – undesirable interaction between the fixed layers and free layer appeared unavoidable. The result was an early biasing of the magnetization state of the free layer before the input from the MQCA wire could reach it. The Freescale commodity MRAM part avoids this problem in three ways:

- Two antiparallel fixed layers were used in close proximity to each other, which strongly coupled the fringing fields of the fixed layers to each other and prevented them from reaching the free layer to any great extent.

- The design utilizes two antiparallel free layers as well which switch together, further reducing the impact of fringing fields from the fixed layers.

- The toggling switching system ensures that biasing problems are minimized, because while the free layers are settling, the fixed layers have also been displaced somewhat and thus affect the easy axis magnetizations of the free layers less.

We do not enjoy most of these same benefits in the MEI. We cannot use two antiparallel free layers, because to do so would cause the impact of the neighboring MQCA cell to become meaningless; magnetized in either configuration, the MQCA
cell would have no net effect on the MEI’s free layers. While the toggling switching system produces some of the same reactions in the fixed layers of the MEI as it does in MRAM, the same does not apply to the free layers, and thus the benefit is reduced. We do, of course, use antiparallel fixed layers. Even with these changes, however, designing the MEI’s gap between free and fixed layers to be the same as MRAM’s results in failed designs, the free layers of which bias quickly in the direction antiparallel to the nearest fixed layer. To correct this, it is necessary to widen the gap between free and fixed layers, rendering TMR no longer usable as the maximum thickness of the insulative tunnel barrier can be no more than about 10 Angstrom (1nm) \[^{[Miyazaki and Tezuka (1995)]}\]. At 3nm, the gap is wide enough to mitigate the effects of fringing fields from the fixed layers such that the free layer is almost entirely free of exchange bias introduced by the layer below it.

3.1.3 Proposed Designs and Solutions

Because this switching operation is more delicate than that of an MRAM device, several concerns must be addressed before it can be certain that the MEI will work correctly. The first simple device created in simulation, a free layer composed of permalloy, copper spacer and fixed layer composed of Co-Fe alloy, each 2nm thick, failed immediately and repeatedly, under different testing parameters. Without exception, the free layer became biased in the direction antiparallel to the fixed layer below it and remained magnetized in that direction throughout the simulation, though the input for the neighboring MQCA cells was changed.

One approach tried to solve the biasing problem was to insert a “companion magnet” next to the MEI on the opposite side from the MQCA as shown in
Figure 3.2. Diagram of an older, unsuccessful design using a companion magnet to absorb the fringing fields of the fixed layer.

The rationale behind this approach was that the companion magnet, placed on the same level as the upper fixed layer, would absorb more of the fringing fields from the fixed layer as the lower fixed layer was intended to do, coupling with it antiferromagnetically and reducing the impact of those fields on the free layer. While this approach was somewhat successful, the free layer did not switch reliably and in some cases, distortions in the magnetization of the free layer, apparently caused by the companion magnet, made those results unusable.

Eventually, after much trial-and-error, it became clear that the design must include twin fixed layers, one below the other and antiparallel to each other. This caused the fixed layers’ fields to interact with each other more strongly than they interacted with the magnetization of the free layer. These initial designs failed too, until the fixed layers were placed only a nanometer apart from each other and the free layer was positioned 5 nanometers away from them. The close association of the fixed layers’ fields combined with the free layer’s distance from them enabled the free layer to switch according to the magnetic orientation of its neighboring MQCA cell and kept the fixed layers’ fields interacting with each other rather than the free layer as shown in Figure 3.3.
3.2 Design Description

The final design of the MEI is described as follows.

The device as simulated contains 5 layers of metal, alternating between magnetic and nonmagnetic materials. The top layer is the free layer, a 2nm thick layer of permalloy (20% Ni, 80% Fe alloy). Permalloy is chosen due to the fact that it is an extremely magnetically soft material, meaning that it has a low coercivity and thus its magnetization is easily susceptible to change owing to influence from an external magnetic field. (Another, similar metal, known as supermalloy, is even more magnetically soft, but was not chosen due to a desire to introduce a certain amount of conservative “fudge factor” in the design liberties permitted by material choice.) This is followed by a 3nm thick conductive spacer layer. This can be any conductive metal; most extant GMR devices use copper, but other materials such as gold, aluminum and lead have also seen use in experimental devices. After the spacer is a fixed layer composed of CoFe alloy; this is less magnetically soft.

Figure 3.3. Sketch of how the fields between layers in the MEI interact with each other. Dotted lines show weak field interaction. Solid lines show strong interaction.
than permalloy and lends itself well to holding its magnetization in the presence of relatively strong MQCA clocking fields. Experiments have demonstrated that the fixed layers return to their original magnetization after being exposed to fields along the hard axis as strong as 200mT, but we will shortly discuss why this is not terribly significant.

The fixed layer is followed by another conductive spacer only 1nm thick; this exists only to set up a strong magnetic interaction with the second fixed layer below it. This layer is also 2nm thick and composed of CoFe alloy. This produces a device which is a total of 10nm thick. Note that a production device would probably share the Freescale MRAM’s solution for maintaining the magnetization of fixed layers in the face of strong, spurious magnetic fields. This consists of a 10nm thick layer of antiferromagnetic IrMn alloy placed underneath the entire MRAM cell which functions as a pinning layer for the fixed layer directly above it. This accomplishes the goal of holding the lowest fixed layer’s magnetization in place, due to the phenomenon known as exchange bias (Nogus and Schuller (1999)). Because one fixed layer’s magnetization is held, even if the device is exposed to a strong magnetic field that removes all of the upper fixed layer’s remanent magnetization in the easy axis, the lower fixed layer will restore it to the correct magnetization thanks to its own pinned magnetization and the strong field interactions between it and the layer only 1nm above it. Experiments have also demonstrated that a “companion” MQCA cell “in front of” the MEI is necessary for reliable operation; we have simulated the device with such a design in mind.

The clocking field is applied to the magnetic material, and the magnetizations of all the layers in the device, including the fixed layers, shift towards the hard axes of the magnet. In the case of the free layer of the MEI, the remanent magnetization
in the easy axis is almost completely removed. This is not so for the fixed layers, however, which only “bend” together somewhat in the direction of the applied clocking field. When the field is removed, the magnetization of the fixed layers “snaps” back to their original antiparallel configurations along the easy axes of the layers. Some of the energy used to change the magnetic vector of the fixed layers remains and ends up magnetizing the fixed layers more strongly in their opposing configuration. (Note that this behavior remained even in field strength tests up to 200mT.) In production MEIs, the device would include an antiferromagnetic layer about 10nm thick below the bottom fixed layer, which would serve both to help protect the fixed layers from magnetizing in incorrect directions and ensure the fixed layers were “stuck” in a configuration that keeps their high-resistance state high.

Note that it was not possible to include the antiferromagnetic layer typical of other GMR and TMR devices in our simulations because the simulator does not support antiferromagnetic materials, however, the fact that the device worked well without the AF layer can only be a positive sign for its future performance with it included. Figure 3.3 and Figure 3.1 illustrate the design, without the antiferromagnetic pinning layer.

3.3 Potential Applications

The most obvious and apparent application for the MEI is a simple output interface with the CMOS “outside world.” In its simplest incarnation, the MEI and its companion cell would be positioned at the end of a wire, in their own clocking zone. The clocking scheme has been outlined in other work (Alam et al. 2007). The timing for the clocking would work much like the potential input
design we discussed in Chapter 2, but in reverse: the MEI clock would “wait” until the wire zone had settled completely, then relax and allow the companion cell and free layer to polarize in the correct directions. While it appears that with this iteration of the design, at least, a separate clocking zone is necessary for the interface to be able to synchronize correctly with the rest of the MQCA logic, this is not a significant drawback. One-quarter of a clock cycle to produce output, in only a few locations on a chip, is a negligible performance drawback.

Another, more intriguing application of this device is as a form of fast interconnect from one portion of the chip to the other. Figure 3.4 is a simple diagram of how this could work. By creating an electrical via in metal from the MEI to an input source on another part of the chip, the MQCA system designer can “skip” clocking zones ahead of the MEI or loop back data to physically “earlier” portions of the chip. Skipping zones has obvious speed advantages, but it could also be used in branch prediction hardware to forward data past clocking zones from the branch predictor to the ALU. Note that most concepts of production MQCA logic are for applications like digital signal processing, which involves very few branches, but nevertheless, this kind of “instant jump” ability conferred by the MEI could expand the potential number of applications for MQCA logic by making the circuitry more flexible.

3.4 Manufacturing Considerations

Care would have to be taken to fabricate an MEI using current CMOS technologies. Note that our design as shown requires 5 layers of variously thick metal to be applied in the same space as 10nm of permalloy (for the MQCA elements). In a production design, the MQCA cells would more likely be 20 or even 30nm
Figure 3.4. Diagram of how a MEI device could be used to forward information through the MQCA clocking "pipeline" (arrow on the right, pointing to the next clocking zone) or backwards through the circuit as a feedback mechanism or for the creation of memory arrays. The "green" or lightly shaded cells are MEI devices or spin-torque/clock-zone input devices.
thick, but this does not change the fact that somehow, either two different materials must be deposited at once or there must be two separate deposit-etch cycles to get the MQCA cells correctly aligned with the MEI.

This process might work as follows:

- Deposit the first, non-permalloy layers for the MEI
- Etch around the MEI using well-known photolithographic etching techniques
- Deposit the permalloy layer for the MQCA
- Etch around the MQCA
- Use a process like chemical-mechanical planarization to “shave” the permalloy that would extend too high atop the first MEI layers

Note that the last step for depositing the MEI is permalloy, which is what the MQCA devices are composed of as well.

Current fabrication techniques do not permit the kind of guaranteed overlay mask accuracy that would be necessary to make MEIs mass-producible. The 2007 ITRS lithography roadmap notes that in 2008, with “3 sigma” accuracy, current technology should place overlay accuracy at about 11.3nm (ITR (2007)). This, of course, is almost precisely the distance between MQCA elements, and between MQCA elements and the MEI. This means that it is possible to irradiate a chip with a mask image and be confident that the second masking will be within the same boundaries to within 11.3nm. This would not be acceptable for fabrication, as an attempt could result in the MEI and MQCA elements actually touching rather than being separated by space.

The good news, however, is that it is not necessary to have this accuracy immediately. Research is ongoing in magnetic logic devices and there are many
unsolved problems (and there exists much more interesting research!) to address before system designers can seriously look at including MQCA devices in their designs. The ITRS also states that by 2012, 2.9 nm overlay accuracy should be possible. By 2021, accuracy should be within 2.5 nm. These predictions are given with the “manufacturable solutions exist, and are being optimized” qualification. With 2.5 nm accuracy, the mask for the MEI etch can only move by a maximum of a quarter of the total distance between the cells. The simulations we have conducted in OOMMF were conducted with a 5 nm grid size in the x and y dimensions and worked well; if the mask can be restricted to move less than half of this distance between lithography attempts, we can be reasonably assured that process variations caused by mask inaccuracy will not be a “deal-breaking” problem. This gives us a fair amount of confidence that the necessary technology for fabrication will be available to MQCA system designers when they begin building real systems. In addition, for research purposes, though repeated mask accuracy is not statistically guaranteed, it will generally be possible with a high rate of success to produce MEI examples that are nearly perfectly aligned, just not on a commercial scale.
In this chapter, we present the choice of the OOMMF micromagnetic simulation package and its utility for evaluating MEI designs. We also detail the choices for simulation parameters, reasons for those choices, and final results, as well as some problems that were encountered during the evaluation process which revealed some important lessons for nanomagnetic device design.

4.1 The OOMMF Micromagnetic Simulator

OOMMF is a software package developed by the National Institute for Science and Technology for performing single-threaded, micromagnetic calculations. It uses a Landau-Livshitz-Gilbert algorithm to mechanistically simulate the relaxation (reduction of energy state to its lowest level) of magnetic spins in a 2D or 3D mesh. It is capable of applying external magnetic fields to a piece, or several pieces, of magnetic material, defined using a series of bitmap image files. After the fields have been applied, it can then remove the fields and produce the result when the spins in the magnetic material return to their ground energy state. This capability is useful for simulating devices such as MRAM, the MEI, and MQCA cells because this is precisely how we can simulate bit and digit line fields and clocking fields, respectively.
Figure 4.1. Image of the mmDisp data visualization portion of the OOMMF micromagnetic suite running in X Windows under Mac OS X. The data reveal a working MQCA 7 cell wire terminating in a working MEI.

OOMMF also presents a variety of ways of collecting data, but the most commonly-used method for this work is simple observation of the graphic output produced by the mmDisp component of the application. Figure 4.1 shows a typical mmDisp window running in Mac OS X Leopard 10.5.2. The size of the arrows showing the magnetization vector at variously sampled points in the simulation is user-configurable, as are most other parameters of display. The individual “pixels” visible in the display are color-coded according to the angle of their magnetization; this is useful in our work for observing patterns of magnetization and determining which are desirable and which are undesirable. Note that the display shows the user only a “slice” in the z-dimension of the simulation. The slice shown is adjustable, but the display can also be rotated to show the material being simulated in a z-y or z-x plane rather than simply x-y.
Figure 4.2. Image from the mmDisp data visualization portion of the OOMMF micromagnetic suite, showing the magnetization data and total field data of the same portion of a simulation at the same time step. Note the strong magnetic field interaction between the fixed layers.

At the bottom of the image, Figure 4.2 gives an example of a zoomed-in display of the MEI and a few neighboring MQCA elements in cross-section. At the top of the image, it gives an example of the same piece of magnetic material, but is set to display the total field present due to the magnetic flux present inside the magnets. This kind of information is especially valuable when attempting to troubleshoot problems with the free layer becoming biased in an undesirable direction due to influence from the fixed layer below it. In this example, note the strong interaction between the top and bottom free layers and much smaller interaction between the topmost fixed layer and the free layer above it. This is desirable behavior brought about by the close proximity of the fixed layers and relative distance of the free layer.

Because OOMMF is only a magnetic simulator, we unfortunately cannot use it to determine what the electrical properties of the multilayer MEI we have discussed in this thesis are. Software packages capable of this kind of analysis are
significantly more costly than the investigator can afford – especially compared to OOMMF, which is Free Software. However, we can be certain to a reasonable degree that it will share many of the same electrical properties as existing devices built along the same lines; thus, the absolute resistance demonstrated by the device should be in the range of 16-20KOhm, the current passing through it will be similar to that of existing GMR magnetic hard drive read heads, etc.

Before we address simulation results directly, it is necessary to explain what precisely the images shown represent. When a simulation takes place, the bitmap layers that make up the 3-dimensional representation of the material being simulated must be discretized into a 3D grid. Each dimension may have a different granularity or resolution in terms of nanometers. The simulator then begins solving the LLG (Landau-Livshitz-Gilbert) equations between the grid cells to determine what the lowest energy state between them is. The arrows shown inside the colored pixels denote a sampled vector of magnetization (or, in other cases, the vector of the magnetic field under consideration) in the area of the grid cells near to them. Desirable behavior, in the case of the MEI, is alternating “up” and “down” magnetic vectors in each MQCA cell and, finally, the free layer of the MEI itself. These vectors must also nullify completely enough to switch in the opposite direction when the clocking field is applied, the input is changed, and the clocking field is relaxed. A “failed” design does not exhibit this behavior.

4.2 Simulation Parameters and Setup

4.2.1 Material Parameters

All simulations shared the following parameters: 10nm separation between the MQCA cells, cells with dimensions of 60nm in the “x” dimension by 90nm in the
“y” dimension by 10nm “thick” in the z dimension, an OOMMF discretization grid of 5x5x1, one “sudden” time step per change in state of the simulation, a 200mT input field for the first MQCA element, $3.5 \times 10^{-6}$ as the value for the magnetocrystalline anisotropic constant for CoFe alloy \cite{zhao2006}, and used the same semi-systolic clocking scheme, which we will detail below.

We chose these parameters after studying how MQCA devices interacted with each other without a MEI in use. Ten nanometers of separation between cells is both physically possible and desirable from an operational standpoint; repeated experimentation has shown (somewhat predictably) that the closer together two MQCA elements are, the better they interact, the more reliably they switch in response to changes in input, and the less strong of a clocking field is needed to cause their magnetizations to null completely to their hard axes.

The 60x90 size for MQCA cells has been determined experimentally to be a good “compromise” between the high aspect ratio needed to encourage the magnetization of the cells to settle strongly in either of the easy axis directions and the low aspect ratio which encourages the cells to switch easily with as little force from the clocking field as possible. When the aspect ratio of the cells is too high, the requisite clocking field to null their logical states by pushing their magnetizations in the direction of the hard axis becomes prohibitively strong. Conversely, when the aspect ratio is too low, the cells lose their tendency to polarize strongly in either an up or down direction, and it becomes possible for data to be lost to uncertain magnetic states. The 10nm thickness was chosen based on other reference designs (mostly MRAM and GMR magnetic hard drive read head designs) which utilized similar thicknesses. It also serendipitously turned out to be convenient for simulation, as it became possible for all the layers to be
generalized to thicknesses in increments of 1nm.

The discretization grid size, which can be thought of as the granularity or “resolution” of the simulation, was chosen for a number of reasons. Three-dimensional simulations of high granularity can take an inordinate amount of time to complete in OOMMF, as long as a month or more for large simulations of parts e.g. 500x500x10nm, if the granularity chosen is around 3nm. While 3x3nm is suitable for 3D simulations of MQCA that are effectively 2D (i.e. simulations run with the 3D OOMMF engine but which are 2D in nature), 3x3x1nm simulations take quite a bit longer, on the order of weeks, for larger devices.

Choosing the 5x5 x by y grid size served two purposes. First, it allowed the simulations to run in a much shorter length of time (usually no more than half a day) than would be permissible with higher-resolution simulations, and second, it introduced a certain amount of conservative tolerances into the experimental work. It stands to reason that the higher a granularity or resolution a simulation one runs to test a design, the more accurate it will be and thus less sensitive to faults caused by an inaccurate rendering of the conditions of the test. We have seen this proven out in preliminary work to this thesis; simulations that fail to operate correctly at 5x5 grid size sometimes succeed when the granularity is increased to 4x4 or 3x3. Thus, if a test functions correctly at 5x5 granularity, we can say with a higher degree of confidence that it will be successful in the “real world” when actually implemented than if we ran all tests at a higher granularity. The 1nm z-dimension grid size was unavoidable; since our multilayer MEI has one layer (the conductive spacer between the two fixed layers) which is 1nm thick, we needed a 1nm resolution in the z-dimension to represent it accurately. Note that OOMMF can use independent numbers for each dimension as long as the
number of simulation cells (not MQCA “cells”) is divisible by each grid size in the
dimension in question. One can, for example, run a simulation with a 3x4x5 grid
if the overall size of the simulation is 90x40x50.

The time step parameter was another decision made for the sake of speed of
simulation and conservatism in tolerances. In the tests performed in Imre’s work,
the clocking field was relaxed over the course of 30 seconds. This enables the
magnetizations of the MQCA cells to settle in a very organized, reliable manner
with no magnetic resonance caused by the magnetizations “snapping” back into
positions too quickly. If we were to run an OOMMF simulation which lowered
the clocking field over a 30 second time span, the simulation would easily take
years or possibly centuries to complete. Instead, we chose the default OOMMF
OxsTimeDriver (the object which manages the progress of the simulation) behav-
ior, which performs a “square-wave” instant-on, instant-off management of the
clocking field. This is actually a worse case than what would realistically happen
in a production device; it is more or less impossible to instantly produce a (for
example) 50mT clocking field and instantly turn it off. This is due to capacitance
and inductance effects in wires. In addition, a clocking field rising and falling
pattern closely matching a sine wave has been shown to produce much more de-
sirable results in tests than that matching a square wave. This means that with
the use of this “harsher” clocking system, we intentionally make it more difficult
to obtain correct results with a worst-case switching time.

The strength of the “input field” is actually mostly immaterial for these sim-
ulations. It serves only to produce a strong magnetization of the first MQCA cell
and produces no effects down the wire apart from how the magnetizations match
the input cell. We chose 200mT simply because we could be assured a field of that
strength would quickly and reliably flip the magnetization of the first cell during
the simulation.

While quite a bit of research was necessary to determine exactly what the
magnetocrystalline anisotropy of CoFe alloy is (different resources had different
determined values, but all within the same order of magnitude), some experimen-
tation has revealed that changing the value does not appear to affect simulation
results in any appreciable way. While existing MRAM designs, for example, have
carefully annealed fixed layers to ensure that their “easiest” magnetization axis is
in the desired direction, such a measure appears not to be necessary in the MEI’s
design. It may be that the effect of the annealing is more noticeable when one
layer is pinned with the underlying antiferromagnetic layer; as it is, the fixed lay-
ers “scissor” together and snap back into position without any other undesirable
changes. Note that we did not include a magnetocrystalline anisotropy value for
permalloy because the value is almost zero (it has no preferred magnetization due
to crystalline structure).

4.2.2 Clocking Parameters

The clocking scheme used is the same as in other QCA systems. Table 4.1
shows the on-off pattern of the two clocking zones found in all the simulations we
ran.

We can be assured that the clock field arrangement is possible because, due to
the way switching works in MQCA, it is possible to have any arbitrary number
of clock zones before a zone. Additionally, there is no reason the MEI could not
have its own zone, if necessary. As it turned out, the device functions best with
one MQCA cell before it in the zone (in other words, the design proceeds as:
TABLE 4.1

Clocking of MQCA and MEI Elements in Simulation. Note that the input value was changed between stages 2 and 3.

<table>
<thead>
<tr>
<th>Stage</th>
<th>First Clock Zone</th>
<th>Second Clock Zone</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>On</td>
<td>On</td>
</tr>
<tr>
<td>1</td>
<td>Off</td>
<td>On</td>
</tr>
<tr>
<td>2</td>
<td>Off</td>
<td>Off</td>
</tr>
<tr>
<td>3</td>
<td>On</td>
<td>On</td>
</tr>
<tr>
<td>4</td>
<td>Off</td>
<td>On</td>
</tr>
<tr>
<td>5</td>
<td>Off</td>
<td>On</td>
</tr>
</tbody>
</table>

zone boundary, MQCA cell, MEI, end of zone), presumably because this cell is given a chance to hold its polarization until the remainder of the wire has settled and then as it relaxes, polarize the free layer of the MEI in the desired direction. Note that this kind of behavior illustrates the fact that the MEI does not at all behave magnetically like an MQCA cell. When experiments were run with the MEI in its own clock zone, the magnetic “pull” from the MEI’s layers being pushed in the direction of their hard axes was not enough to correct the timing problems mentioned in Chapter 2 at the MEI end of the wire. What resulted was incorrect output from the wire and the MEI’s free layer simply settling antiparallel to however its uppermost fixed layer was set.

It is also notable that 50mT is a fairly strong field compared to that needed to switch MQCA cells in simulations only of MQCA devices. Part of the appeal of MQCA is its potential for very low power consumption (Alam et al. (2007)). 48
However, the added power consumption to account for a potentially stronger field should be largely negligible due to the fact that not many MEI devices would be needed in any given MQCA system. We have applied 50mT of magnetization to each of the fixed layers in antiparallel vectors to start the simulation; this is a conservative design as it is possible to magnetize both layers to a greater degree with processes such as annealing (Fuke et al. (1997)).

4.3 Problems and Solutions in Simulation Evaluation

Some problems were encountered when an attempt was made to “feed” the MEI with MQCA wires longer than three or four cells. With longer wires, the simulation would revert to behavior shown with older test designs, showing the MEI’s free layer simply setting itself to a magnetic orientation antiparallel to its nearest fixed layer and staying in that orientation throughout the simulation. This appeared to be simply a problem with timing: the influence of the small biasing effect from the fixed layer caused the part of the wire closest to the MEI to settle to a new state more quickly than the part of it closest to the simulated electrical input, as shown in Figure 4.3. This problem was eventually eliminated by introducing multiple clock zones to the wire. By clocking a piece of wire in two zones, it was possible to keep the MEI’s smaller segment of wire in the “null” logic state while the input wire with its simulated electrical input settled into the correct state.

Another issue encountered was persistent misalignment in wires longer than about four or five cells. An “up, down, up, up, down, up, down” logic pattern, for example, would persist even after the logical input was changed at the beginning of the wire. In shorter wires, some cells would “stick” in an intermediary
Figure 4.3. Graphic representation of a wire terminating in a MEI device. Note that while the left side of the wire is polarizing correctly, the MEI’s free layer is being biased slightly in the upward direction by the fixed layer beneath it. This causes the wire not to switch properly, and ultimately the MEI as well.

“curved” state rather than polarizing up or down. These problems would sometimes disappear when the granularity of the simulation was increased, but this “fix” was not consistent. Eventually, it was noticed that two of the MQCA cells were closer together than the others. This usually does not produce much of a timing issue in the “usual” set of MQCA simulations; these are run at a 3x3nm grid resolution and a small amount of “shift” in the MQCA cells does not make much of a difference. However, the MEI simulations’ 5x5nm x-y resolution created a discretization problem in the simulations. A single simulation cell of shift resulted in a distance change in the MQCA cells from 10nm apart to 5nm apart.

Figure 4.4 shows an example of this discretization problem causing the third cell in a short wire to behave incorrectly at the end of a clocking stage.

Thus, fixing this problem (simply by shifting the MQCA cells around somewhat in the bitmap image which the simulator used to describe them) taught us an important lesson: while differences in cell separation of a few nm at 15nm separation or even 10nm did not appreciably affect performance, the closer the cell separation got to “touching,” the more extreme the reaction. In the case of
Figure 4.4. Graphic representation of the discretization error in a 4-cell wire terminating in an MEI. Note that in this case, the third cell, which is too close to the second, sticks in an intermediary state. The block of magnetic material at the end serves only as a (ultimately unnecessary) way of managing timing in the wire.

this “stuck-at” error that the discretization problem caused, it would cause two cells to behave as one, making them “stick” in whatever direction they polarized first. This informs the MQCA system designer that while close spacing between cells is desirable for lower-power operation, the closer the spacing, the greater the potential sensitivity to defects that vary the spacing between cells.

Unfortunately, since the requisite software was not available, it was not possible in this project to evaluate exactly what the change in magnetoresistance would be for a spin-valve device of this type. An examination of the MEI in Figure 4.5 reveals that when the free layer’s magnetization is in the “down” orientation, the angle of the vector is not quite as parallel to the y axis as it is in the “up” orientation. This is no doubt due to the influence of the fixed layer below it. The ideal case for the GMR effect is magnetic layers directly in opposition to each other; some amount of deviation from this will no doubt affect the level of magnetoresistance exhibited by the device. It will be necessary to characterize this deviation quantitatively before trying to deploy the MEI in working MQCA systems.
4.4 Results

The final set of successful tests was run with a 50mT clocking field on both the 6-cell wire feeding the MEI and the MEI itself. It was found that with a simple two-stage clocking arrangement on the interface and its wire, timing problems wherein the MEI prematurely biased the wire were eliminated. We omit simple single-cell examples here for brevity; it was uniformly much easier to get shorter wire segments working correctly even with the least beneficial simulation parameters, and a one-cell-long, input-only wire is the shortest example one could construct. Parameters for the final battery of successful tests can be found in Table 4.2.

Note that we define “working” here as “free layer of the MEI switches from one state to the other between input states when the clock is applied and relaxed.”

We learned several things from these experiments. First, the clocking field for the MEI must be relatively high compared to the extremely low field strengths we have previously observed working in MQCA (3-5 mT in Alam et al. (2007)). As we discussed earlier, this is not much of a problem for the MQCA system designer due to the relatively small number and small area of the clocking zones necessary for output. Second, the MEI appears to need a “neighbor” MQCA cell just before it and after the clock zone transition boundary in order to respond to the clocking field properly. Extending the length of the MEI’s clock zone to more than two elements (that is, the MEI itself and one MQCA cell) uniformly resulted in incorrect output. This appears to be because the MEI, which does not share the same magnetic characteristics as the MQCA cells, needs something next to it to help “force” it to null the magnetization of its free layer to zero while the input wire’s clock field is relaxing. Also, the end of the MQCA wire needs a
TABLE 4.2

Testing Parameters for Various Instances of MEI

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Clock Field Strength</th>
<th>Length of MEI Field</th>
<th>Working?</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>80mT</td>
<td>3</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>90mT</td>
<td>3</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>100mT</td>
<td>3</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>80mT</td>
<td>4</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>90mT</td>
<td>4</td>
<td>No</td>
</tr>
<tr>
<td>6</td>
<td>100mT</td>
<td>4</td>
<td>No</td>
</tr>
<tr>
<td>7</td>
<td>80mT</td>
<td>1</td>
<td>No</td>
</tr>
<tr>
<td>8</td>
<td>90mT</td>
<td>1</td>
<td>No</td>
</tr>
<tr>
<td>9</td>
<td>100mT</td>
<td>1</td>
<td>No</td>
</tr>
<tr>
<td>10</td>
<td>80mT</td>
<td>2</td>
<td>Yes</td>
</tr>
<tr>
<td>11</td>
<td>70mT</td>
<td>2</td>
<td>Yes</td>
</tr>
<tr>
<td>12</td>
<td>50mT</td>
<td>2</td>
<td>Yes</td>
</tr>
<tr>
<td>13</td>
<td>40mT</td>
<td>2</td>
<td>No</td>
</tr>
</tbody>
</table>
“solid” piece of magnetic material to hold the “tail” end of the wire in its nulled state. Third, the final result of the 40mT simulation was interesting: while the MEI’s magnetization did not switch correctly upon exposure to the clocking field, it actually polarized in the “more difficult” direction (parallel to the uppermost fixed layer rather than antiparallel) in both input phases. This suggests that with some additional engineering and experimentation, it may be possible to obtain good results with 40mT clocking fields or even lower-strength fields.

Figure 4.5 shows the progress from stage to stage of the successful 50mT test.

Some of the undesirable biasing of the free layer from the fixed layer below it is visible in the MEI at the end of the wire. In any GMR device it is incumbent upon the designer to ensure that fringing fields from other parts of the device do not interfere with the free layer; in this case the switching of the MQCA element directly to the left of the MEI keeps the fringing fields from affecting it too strongly.

The preceding image shows a correctly-functioning 6-cell wire with one additional element after it, the MEI. It appears as though it were just another MQCA cell because it is of the same dimensions. All that is visible in the image is one z-slice of the total part. Appendix A describes how the simulator “sees” the magnetic material we simulated in greater detail.
Figure 4.5. Series of images of the successful MEI test, from one stage to the next. z-slice chosen in this case was the 9.0nm slice. The MEI and its companion cell are the two elements at the end of the wire; the clocking boundary is directly before them.
5.1 Conclusion

A variety of technologies have been explored in recent research to replace or supplement standard CMOS technology. In this thesis we have explored a promising technology to not only bridge a potential new way of doing digital logic in MQCA with standard CMOS, but also potentially significantly enhance that new technology with speed and flexibility.

We have investigated the spin-valve design of the MEI, which has been explored previously in MRAM and hard drive technology, and have found it lends itself well to interaction with magnetic QCA parts. The free layer of the MEI, given the right operating conditions, can align itself in an antiparallel manner to neighboring MQCA elements and change the MEI’s resistance according to how the free layer’s magnetization is biased by the MQCA elements after being exposed to the clocking field.

Design complications that arose during the evaluation process were dealt with in a systematic way, by applying lessons learned from existing technologies and ascertaining which changes to the design overcame the problems of fixed layer fringing fields and timing issues. Important lessons were learned along the way regarding how to manage timing concerns in MQCA system design as well as building systems with heterogenous components (such as MQCA cells and MEIs).
Currently, the requisite clocking field to enable a MEI to switch correctly is relatively strong at 50mT, but we are reasonably confident first that strong clocking fields only for the interface are not a significant problem for the MQCA designer and second that some reduction in field strength will be possible with further engineering and exploration of MQCA technology. Thus, the future for this technology seems relatively bright.

It is important to note that with the introduction of the MEI as a building block of MQCA, there now exists no practical barrier to the implementation of, at the least, experimental MQCA computing devices that can be deployed in larger-scale experimental systems. If we know that there exist methods for input in the form of spin-torque MRAM and dedicated input clocking zones, methods for clocking in the form of ferrite-yoked conductive plates, and methods for output in the form of the MEI, we can conclude that the building block set for MQCA systems is now complete. If fabrication hurdles involving the MEIs multilayer structure can be overcome, MQCA will become the only viable nanotechnological computing technology available to system designers out of the many proposed technologies. It is low-power, potentially quite fast, scales much better than CMOS, and available for use in the next few years.

5.2 Future Work

As we noted earlier, some work remains in the evaluation of the MEI as a viable interface technology for MQCA and CMOS.

Quantification of the behavior of the device would also be desirable for future implementation studies. Exact measurements of the ratio of the angle of magnetization of the free layer to the resistive qualities of the device would be necessary
to begin implementation, for example.

We have left mostly unaddressed the question of the sensing circuitry responsible for determining the logical state of the device. This is because, in part, the sensing circuitry is a solved problem. Freescale’s MRAM sensing circuitry was itself based on prior work in magnetic hard drive read head technology. The primary barrier to accurate sensing with a change in magnetoresistance of 5% will be the quality of the process technology used to create the devices. Essentially, this means that the process deviation between the MEIs and their reference bits must be commensurately small as one seeks to discern smaller and smaller changes in MR. Whether or not this is possible is an open question requiring some further investigation, but we are reasonably confident solutions will present themselves in the future based on predictions of process technology by ITRS.

Finally, some refinement of the physical structure of the device will almost certainly be necessary before deploying it. By necessity of the limitations of OOMMF, we were limited to simulating layers of metal that were nanometers in thickness; no greater granularity in the z-dimension was permissible. Meanwhile, many spin-valve designs, Freescale’s inclusive, are often cited as having layer thicknesses in Angstroms. We are optimistic that future work to study precisely what layer thicknesses, areas, and other geometry work best in the MEI will reduce impingement of the free layer by fixed layers’ fields, improve change in magnetoresistance, and help characterize exactly what fabrication technology is necessary for the mass-production of MQCA devices with built-in CMOS interfaces.

Fabrication of the device will enable designers to study real-world MQCA systems without depending on bulky, slow MFM for output characterization. It will also produce new and exciting possibilities for circuit design. Physical realization
is the next, necessary, logical step for MQCA I/O research.
Appendix A: OOMMF simulation parameters and Tcl source code

# MIF 2.1
# Developed by Jarett DeAngelis
# 1/4/08
# Edited 3/1/08 for comments for clarity
# 7cell-fixbmp-len2.mif2

# constants
set PI [expr {4*atan(1.)}]
set MU0 [expr {4*$PI*1e-7}]

# Note that the MQCA elements in this simulation
# are represented by 5 layers of permalloy of varying thickness.

# This is the bottom layer of CoFe alloy.
# It is the bottom fixed layer of the device.
Specify Oxs_ImageAtlas:layer1 {
xrange {0 495E-9}
yrange {0 100E-9}
zrange {0E-9 2E-9}
image longtest.ppm
viewplane xy
colormap {
white nonmagnetic
black permalloy
red cobalt
}

# This is the 'empty' spot in the stack which represents the
# conductive spacer between the fixed layers.
Specify Oxs_ImageAtlas:layer2 {
  xrange {0 495E-9}
yrange {0 100E-9}
zrange {2E-9 3E-9}
  image longtest-empty.bmp
  viewplane xy
  colormap {
    white nonmagnetic
    black permalloy
  }
}

# Top fixed layer, also composed of CoFe. Note that the colormap
# for the cobalt is different because we have informed the simulator
# that the magnetocrystalline anisotropy is set in the opposite direction
# from its lower companion layer.

Specify Oxs_ImageAtlas:layer3 {
    xrange {0 495E-9}
    yrange {0 100E-9}
    zrange {3E-9 5E-9}
    image longtest.ppm
    viewplane xy
    colormap {
        white nonmagnetic
        black permalloy
        red cobalt2
    }
}

# This is the 3nm thick Cu spacer between the fixed layers and
# free layer.

Specify Oxs_ImageAtlas:layer4 {
    xrange {0 495E-9}
    yrange {0 100E-9}
    zrange {5E-9 8E-9}
    image longtest-empty.bmp
    viewplane xy
    colormap {
        white nonmagnetic
    }
}
black permalloy
}
}

# 2nm thick permalloy free layer at the top of the stack
Specify Oxs_ImageAtlas:layer5 {
  xrange {0 495E-9}
yrange {0 100E-9}
zrange {8E-9 10E-9}
  image longtest-permalloy.bmp
  viewplane xy
  colormap {
    white nonmagnetic
    black permalloy
  }
}

# Input field atlas (physical dimension specification for field)
Specify Oxs_BoxAtlas:field1atlas {
xrange {4E-9 68E-9}
yrange {4E-9 97E-9}
zrange {0 10E-9}
}

# First clock field, for wire
Specify Oxs_BoxAtlas:clock1atlas {
  xrange {2E-9 350E-9}
  yrange {2E-9 88E-9}
  zrange {0 10E-9}
}

# Second clock field, for output stack
Specify Oxs_BoxAtlas:clock2atlas {
  xrange {355E-9 495E-9}
  yrange {2E-9 88E-9}
  zrange {0 10E-9}
}

# Glues everything together
Specify Oxs_MultiAtlas:partatlas {
  atlas :layer5
  atlas :layer4
  atlas :layer3
  atlas :layer2
  atlas :layer1
  xrange {0 495E-9}
  yrange {0 100E-9}
  zrange {0 10E-9}
}
# Specifies granularity of simulation
Specify Oxs_RectangularMesh:mesh {
    cellsize {5e-9 5e-9 1e-9}
    atlas :partatlas
}

Specify Oxs_Exchange6Ngbr:exchange {
default_A 0
atlas :partatlas

A {
    cobalt cobalt 12E-12
    cobalt2 cobalt2 12E-12
    permalloy permalloy 13E-12
}
}

Specify Oxs_Demag {}
default_value 0.0
values {
    cobalt 0.35
}
}
axis {0 1 0}

Specify Oxs_UniaxialAnisotropy:CoFeAnis3 {
K1 { Oxs_AtlasScalarField {
    atlas :layer4
    default_value 0.0
    values {
        cobalt2 0.35
    }
}
axis {0 -1 0}
}

# These are 'dummy' values for the external clocking field,
# which is really handled by the 'Direction' procedures below.
# This set of values really only serves to let the simulator
# know that we expect a total of 6 time periods.
Specify Oxs_UZeeman:extfield0 [subst {
    comment {Field values in Tesla; scale to A/m}
multiplier [expr {1/$MU0}]

Hrange {
    {0 0 0 0 0 0 1}
    {0 0 0 0 0 0 1}
    {0 0 0 0 0 0 1}
    {0 0 0 0 0 0 1}
    {0 0 0 0 0 0 1}
    {0 0 0 0 0 0 1}
}
]

Specify Oxs_StageZeeman:field1 {
    script Field1Spec
}

Specify Oxs_StageZeeman:clock1 {
    script Clock1Spec
}

Specify Oxs_StageZeeman:clock2 {
    script Clock2Spec
}

proc DirectionPermalloy { stage } {
    if {$stage < 3 } {return 0.200}
    if {$stage >= 3 } {return -0.200}

proc DirectionClock1 { stage } {
    if {($stage == 0) || ($stage == 3)} {return 0.050} \
    else {return 0}
}

proc DirectionClock2 { stage } {
    if {($stage == 0) || ($stage == 1) || ($stage == 3) \ 
        || ($stage == 4)} {return 0.050} else {return 0}
}

proc Field1Spec { stage } {
    global MU0
    set spec Oxs_AtlasVectorField
    lappend spec [subst {
        atlas :field1atlas
        multiplier [expr {1/$MU0}]
        default_value {0 0 0}
        values {
            field1atlas {0. [DirectionPermalloy $stage] 0.}
        }
    }]
    return $spec
}
proc Clock1Spec { stage } {
    global MU0
    set spec Oxs_AtlasVectorField
    lappend spec [subst {
        atlas :clock1atlas
        multiplier [expr {1/$MU0}]
        default_value {0 0 0}
        values {
            clock1atlas {[DirectionClock1 $stage] 0. 0.}
        }
    }]
    return $spec
}

proc Clock2Spec { stage } {
    global MU0
    set spec Oxs_AtlasVectorField
    lappend spec [subst {
        atlas :clock2atlas
        multiplier [expr {1/$MU0}]
        default_value {0 0 0}
        values {
            clock2atlas {[DirectionClock2 $stage] 0. 0.}
        }
    }]
}
Specify Oxs_RungeKuttaEvolve:evolver {
    do_precess 1
    gamma_LL 2.21e5
    alpha 0.5
}

# Some materials constants are defined in the code here.
Specify Oxs_TimeDriver {
    basename 7cell-fixbmp-len2/7cell-fixbmp-len2
    vector_field_output_format {binary 4}
    scalar_output_format %.15g
    evolver :evolver
    mesh :mesh
    stopping_dm_dt 12.174983010168182
    stage_count 6
    Ms {Oxs_AtlasScalarField {
        atlas :partatlas
        values {
            universe 0
            nonmagnetic 0
            permalloy 860E3
        }
    }
}
cobalt 1.38E6

cobalt2 1.38E6

} } }

m0 { Oxs_AtlasVectorField {
atlas :partatlas
default_value { 1.0 0.0 0.0 }

values {
cobalt { 0.0 0.050 0.0 }

cobalt2 { 0.0 -0.050 0.0 }

}}

}


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