A model for the behavior of magnetic tunnel junctions

by

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CHAPTER 1. INTRODUCTION

Rationale

A magnetic tunnel junction is a device that changes its electrical resistance with a change in an applied magnetic field. A typical junction consists of two magnetic electrodes separated by a nonmagnetic insulating layer. The magnetizations of the two electrodes can have two possible extreme configurations, parallel and antiparallel. The antiparallel configuration is observed to have the higher measured resistance and the parallel configuration has the lower resistance.

To switch between these two configurations a magnetic field is applied to the device which is primarily used to change the orientation of the magnetization of one electrode usually called the “free” layer, although with sufficiently high magnetic field the orientation of the magnetizations of both of the electrodes can be changed.

The most commonly used models for describing and explaining the electronic behavior of tunnel junctions are the Simmons model and the Brinkman model. However, both of these models were designed for simple, spin independent tunneling. The Simmons model does not address the issue of applied magnetic fields nor does it address the form of the electronic band structure in the metallic electrodes, including the important factor of spin polarization. The Brinkman model is similar, the main difference between the two models being the shape of the tunneling barrier potential between the two electrodes. Therefore, the research conducted in this thesis has developed a new theoretical model that addresses these important issues starting from basic principles.

The main features of the new model include: the development of equations for true spin dependent tunneling through the insulating barrier, the differences in the orientations of the

electrode magnetizations on either side of the barrier, and the effects of the density of states function on the behavior of the junction. The present work has explored densities of states that are more realistic than the simplified free electron density of states function, and has developed an exact analytic solution for the case of an electron band of finite width. The approach taken in this thesis easily allows extension to cases where the band structure is different on either side of the barrier (known as heterojunctions) which are of greater interest in real magnetic tunnel junction devices rather than the simple, identical band structure devices.

Definitions of Symbols

For clarity, the most common symbols used in this study will be listed below.

$D(E)$ – Density of states

$P(E)$ – Tunneling probability

$N(E)$ – Number of charge carriers

$f(E)$ – Fermi - Dirac function

N_s – Number of electron states

$\hbar = \frac{h}{2\pi}$ - Planck's Constant

k – Boltzmann's Constant

T – Temperature (Kelvin)

m – Magnetic moment

m_e – Mass of an electron

e – Charge of an electron

V – Voltage or potential energy

R – Resistance

J – Current density

J_q - Quantum total angular momentum

A – Area

L – Length

E_x – Variable energy in a band

E_{app} – External applied energy

E_F – Fermi energy

μ - Magnetic permeability

ψ - Wavefunction

ϕ - Barrier height

σ - Electrical conductivity

τ - Relaxation time constant

H – Magnetic field

M - Magnetization

Organization of Thesis

This thesis is organized into five chapters. The contents of these chapters are summarized below.

Chapter 2. Background and previous work

The literature review explains important background information on the fabrication, behavior, and the applications of magnetic tunnel junctions.

Chapter 3. First Principles for Theoretical Modeling

This chapter discusses the basic components of the new theoretical model and builds on them to create a model for the current density, resistance area product, and the magnetoresistance behavior of magnetic tunnel junctions, taking into account factors such as the applied voltage, spin polarization of the electronic band structure, effects of changes in the density of states close to the Fermi energy, and differences in the electron band structure on either side of the tunnel junction.

Chapter 4. Results and Discussion

This chapter provides examples of both “open” (standard free electron) and “closed” (finite width or bound electron) band structures resulting from the new theoretical model. This chapter also applies the new model to explain and interpret measurement data and discusses the results. Adjustments are made in order to fit the model to the data. The results of this model are then compared to the Simmons model, and it is shown that the relatively simple extensions of the tunnel junction model developed in this thesis have significant advantages over previous models.

Chapter 5. Conclusions

A brief summary of the study is given along with the benefits and the shortcomings of the new theoretical model. A few new additions that should be included in the new theoretical model are included in the future research section of this chapter.

Appendix

The Appendix lists published work by the author as part of the research undertaken for this thesis as well as a full analytic solution of the important equations in the new theoretical model.

CHAPTER 2. BACKGROUND AND PREVIOUS WORK

Magnetic tunnel junctions consist of two ferromagnetic electrodes separated by a non-magnetic insulating layer, usually an oxide. When a current is passed through these layers, perpendicular to the plane of the layers, a resistance is measured which depends upon the magnetic orientations of the two ferromagnetic electrodes in relation to each other. If the magnetizations of the two electrodes are oriented parallel to each other the measured resistance is normally found to be lower than if they are oriented with their magnetizations antiparallel to each other. This is illustrated in Fig. 2-1.

Fig. 2-1. Illustration of the magnetization directions and their relative resistances.

An applied magnetic field of sufficient strength can change the orientation of these magnetization directions. If both of the magnetic layers are originally in a parallel configuration with zero applied magnetic field then the application of a field to two identical electrode materials will cause the magnetizations to remain in the parallel configuration; no change in the magnetization of the structure is observed. However, if the switching fields of the two magnetic electrode layers are different, then at switching fields lying typically between the coercivities of the two layers it will be possible to have an antiparallel configuration of the magnetizations and this will cause the measured resistance of the tunnel junction to increase. Differences in the coercivity can be caused by selecting different materials for the two layers

(known as a heterojunction), or by using an antiferromagnetic coupling layer that is exchange coupled to one of the magnetic layers, thereby altering its coercivity. This is the basis for the spin dependent tunneling magnetoresistance effect.

A magnetic sensor can be prepared where the resistance of a magnetic tunnel junction (MTJ) would increase or decrease when an external magnetic field exceeds a certain strength. In addition, the bipolar property of these tunnel junction structures (parallel/low resistance or antiparallel/high resistance) allows a device to be fabricated and used for storage of binary information in magnetic random access memory (MRAM). A low resistance value or a high resistance value is read as a one or a zero (binary) similar to existing RAM technology. Many applications of these magnetoresistive devices exist, including: magnetic memory, magnetic field sensors, and magnetic disk drive read head sensors.

Fabrication

Magnetic tunnel junctions must be fabricated under carefully controlled environments. The process that is used must be able to deposit thin films (on the order of 10-100's of Angstroms) and to deposit them in a uniform manner. For this reason, the fabrication process chosen most often is usually a form of sputtering. Sputtering is a process where the substrate is contained in a chamber and then placed under vacuum. An electric field is set up between the substrate (the medium upon which the junction will be deposited) and the target (the material to be deposited on the surface of the substrate). An ionized gas, usually an inert gas such as Ar, strikes the surface of the target and causes atoms from the target to be ejected from the surface. Sputtering is undertaken in a vacuum (of typically 10^{-7} torr or below) to provide the evaporated atoms of the sputtering material a longer mean free path, which means that the

atoms are able to travel longer distances before colliding with other atoms. Sputtering under a high vacuum also helps to minimize the amount of impurities that are deposited onto the substrate. Silicon is a commonly used substrate for the deposition of thin film materials, due to its low cost and availability in wafers of high purity. A uniform magnetic field can be established across the surface of the substrate when depositing a magnetic material [1] in order to induce magnetic anisotropy within the deposited material, even though the final film is polycrystalline, consisting of randomly oriented grains, or even amorphous, depending on the deposition conditions or if the film is subjected to a post deposition anneal.

Test devices may be fabricated from the thin films deposited on the silicon substrate by using common semiconductor processing techniques such as photolithography. [2]

Photolithography involves placing a thin layer of a chemical called photoresist onto the surface of the material that needs to be patterned. This is then placed under a mask and ultraviolet light is used to transfer the image of the mask on to the surface of the substrate.

Acids or other chemicals are used to remove or etch the exposed photoresist and to reveal the material beneath. With this method it is possible to fabricate devices with known geometrical dimensions with complex structures.

The materials chosen for the magnetic electrodes of the tunnel junction are of critical importance to the overall device structure. The magnetic coercivity of each electrode is an important consideration; when a magnetic field is applied antiparallel to the magnetization orientations of the electrodes the layer with the lower coercivity will be the first layer to change in orientation causing the resistance of the tunnel junction to increase. The resistance will remain at this higher level until the field strength becomes large enough to reorient the

magnetization of the layer with the higher coercivity. Once this occurs the lower resistance value is restored. In all cases the resistances of these devices at high magnetic fields (whether positive or negative fields) will be lower, so that the high resistance value only exists over a finite range of magnetic fields.

Basic Properties

The magnetoresistance of a tunnel junction is calculated by the following equation

$$\frac{\Delta R}{R} = \frac{R_a - R_p}{R_p}$$

where R_a is the resistance when the magnetization of the two electrodes are antiparallel to each other and R_p is the resistance when they are parallel to each other. [3] The magnetoresistance will change with the applied magnetic field as shown in Fig. 2-2.

Fig. 2-2: The magnetoresistance versus the applied magnetic field for a typical magnetic tunnel junction. [4]

The Insulating Layer

A simplified energy band structure of a magnetic tunnel junction is shown in Fig. 2-3.

Fig. 2-3. Energy band diagram of a magnetic tunnel junction. [5]

The above diagram shows two possible configurations of the electron band structure in the magnetic electrodes on either side of the tunneling barrier. The upper diagram shows the electron band structures when the magnetizations in both layers are parallel, while the lower diagram shows the electron band structures when the magnetizations are antiparallel.

When electrons tunnel through the barrier it is difficult to change their spin direction.

Therefore, when spin up electrons tunnel through the barrier they tend to remain spin up, likewise the same can be said about the spin down electrons when they tunnel through the barrier they tend to remain in their spin down state. This determines the differences in the

resistance of the tunnel junction when the relative orientations of the magnetizations in the electrode layers change.

In the parallel configuration the majority electron states (spin up) on both sides of the barrier have their spins in the same direction; the minority electron states (spin down) on both sides of the barrier also have their spins in the same direction. When majority state electrons, which in the upper diagram have a higher density of states, will find that it is relatively easy to conduct through the barrier because the band structure in the final electrode is the same as in the originating electrode.

In the antiparallel configuration the majority electron states on both sides of the barrier have their spins in opposite directions. On the left hand side the majority electron states are spin up, and on the right hand side the majority electron states are spin down. Hence, majority state electrons, which in the lower part of Fig. 2-3 have a higher density of states, will find that it is relatively difficult to conduct through the barrier due to the difference in the band structure in the final electrode. This results in a higher resistance to the electron tunneling phenomena.

To simplify the discussion pertaining to the tunneling properties of the tunnel junction only tunneling from an infinite amount of electron states to an infinite amount of electron states will be discussed. In this way the structure of the band structure does not matter. A schematic diagram of this simplified energy band structure and perpendicular distance through the layers of a tunnel junction is shown in Fig. 2-4.

Fig. 2-4. Energy band diagram of a typical tunnel junction. [6]

Fig. 2-4 is a one dimensional illustration of a tunnel barrier. The vertical axis is the energy axis and the horizontal axis is the distance. In this figure the Fermi levels of the two electrodes may be seen along with the energy barrier, ϕ , which is produced by an insulating material. Common materials used for this insulating layer include Al_2O_3 , AlN , MgO , etc. When a voltage is applied to the junction it will change the relative positions of the Fermi levels on either side of the barrier by, $\Delta E = eV$. (e is the electronic charge and V is the applied voltage) In the classical picture the electrons moving from electrode 1 to electrode 2 would need to have an energy greater than the energy of the barrier, ϕ , in order to pass through the insulator, but in quantum mechanics there is a finite probability that electrons with energies less than the energy of the barrier are able to pass through the insulator and reach electrode 2. This tunneling behavior is usually modeled using the Simmons' theory for tunnel junctions. The general equation for this theory is given below [6]

$$J = J_0 \left\{ \bar{\varphi} \times \text{Exp}(-A\bar{\varphi}^{1/2}) - (\bar{\varphi} + eV) \times \text{Exp}[-A \times (\bar{\varphi} + eV)^{1/2}] \right\}$$

$$J_0 = \frac{e}{2\pi h(\beta\Delta s)^2}$$

$$A = \left(\frac{4\pi\beta\Delta s}{h} \right) \sqrt{2m_e}$$

where the coefficient β is a constant usually taken to be 1, h is Planck's constant, e is the charge of an electron, m is the mass of an electron, and V is the voltage. The barrier in this model is assumed to be a rectangular barrier where the average barrier height is modeled using the following equation.

$$\bar{\varphi} = \varphi - \frac{eV}{2}$$

The barrier height, φ , and width, Δs , are variables which are determined empirically by fitting this equation to experimental data of the current density, J , versus the applied voltage, V . A typical current/voltage curve for a magnetic tunnel junction is shown in Fig. 2-5.

Fig. 2-5. A typical current versus voltage curve for a tunnel junction. Dashed – Simmons's model, Solid – Experimental data[7]

Temperature Dependence

The magnetoresistance of the tunnel junction is found to decrease with increasing temperature. An extension of the Simmons model expands on the tunneling current by including the temperature of the junction. The expanded equation is as follows [8]

$$J(V,T) = J(V,0) \times \left(\frac{\pi B k T}{\sin(\pi B k T)} \right)$$

$$B = \frac{A}{2\phi^{1/2}}$$

where $J(V,0)$ and A are the same quantities as the equations given for the tunneling equation above, k is Boltzmann's constant, and T is the temperature in Kelvin. Typical temperature dependent data from a tunnel junction are shown in Fig. 2-6 (adapted from [9]).

Fig. 2-6. A typical magnetoresistance percentage versus temperature curve for a tunnel junction. [9]

Geometrical Effects

The geometry of the tunnel junction also affects the magnetoresistance/applied magnetic field curve. Fig. 2-7 shows the result for a junction with the same total area but different dimensions.

Fig. 2-7. The magnetoresistance effect of tunnel junctions with different dimensions but the same area. [3]

In this figure it is shown that when the long edge of the junction is aligned with the applied magnetic field the magnetoresistance is large and decreases with deviations from this orientation reaching its lower value when the short edge of the junction is aligned with the magnetic field. This is most likely due to the demagnetizing field which opposes the strength of the applied magnetic field. This demagnetizing field is strongest when the applied magnetic field is aligned with the short edge of a rectangle and is weakest when the applied magnetic field is aligned with the long edge of the rectangle.

Enhancing the Magnetoresistance Effect

For many advanced magnetic tunneling devices, it is important to get the greatest change in resistance with applied field for the environmental and structural working conditions of the tunneling device. One of the most important factors is the exchange coupling of the two

ferromagnetic electrodes. A higher exchange coupling means that the energy needed to disturb the parallel alignment of the magnetizations is higher.

The coupling of the two electrodes are affected by “pin holes” (sections of the device where the two electrodes directly touch each other by passing through small defects in the insulating layer) and by surface roughness of the deposited thin films. These two phenomena are illustrated in Fig. 2-8.

Fig. 2-8. a.) Pin hole, b.) Surface roughness. [10]

The left side of the figure shows a pin hole and the right side is an example of surface roughness. Pin holes generally occur for relatively thin films while surface roughness occurs for thicker films.

A common method to help lower the magnetic field required to switch the alignment of the magnetizations of the electrodes is to pin one of the ferromagnetic layers by using a synthetic antiferromagnet. [10] This process causes the coupling between the two main ferromagnetic electrodes to decrease. When coupling an electrode to a synthetic antiferromagnet, the hysteresis loop is shifted by an amount that is equal to the exchange field. The structure of an antiferromagnetically pinned tunnel junction is shown in Fig. 2-9.

Fig. 2-9. A typical magnetic tunnel junction structure with one layer pinned by an antiferromagnet. [10]

Applications

MRAM

Many magnetic tunnel junctions may be arranged in an array and each junction may be electrically controlled to form a magnetic memory device. A typical magnetic memory or MRAM (magnetic random access memory) chip would look similar to the following which is manufactured by Honeywell.

Fig. 2-10. MRAM device developed by Honeywell. [11]

This chip consists of many MRAM bit cells. The magnetization of each of these cells can be either parallel or antiparallel causing a computer equivalent of a one or a zero. A typical MRAM bit cell is illustrated in Fig. 2-11.

Fig. 2-11. MRAM bit cell. [12]

This cell consists of a diode connected in series with a tunnel junction. These devices are interesting due to the nonvolatile state of their magnetization (which means that the data does not have to be constantly refreshed) and their radiation hardness. Radiation has little effect on the orientation of the magnetizations of a magnetic tunnel junction, unlike conventional semiconductor memory which is susceptible to degradation as a result of radiation induced electron-hole pairs which can change the stored information from a one to a zero or vice versa. Both of these concerns, which are major problems with the common semiconductor based memory chips, can be overcome through the use of magnetic tunnel junctions.

SENSORS

In many cases it is advantageous for magnetic field sensors to have small dimensions and a high sensitivity to the magnetic field being measured. However, with sensors the output voltage is usually measured as the applied magnetic field changes and the current through the device is kept constant. A magnetic tunnel junction field sensor manufactured by Nonvolatile Electronics, Inc. is shown in Fig. 2-12.

Fig. 2-12. A magnetic field sensor from NVE. [10]

DISK DRIVE READ HEAD APPLICATIONS

Magnetic tunnel junctions show promise as magnetic read heads for disk drives because of their ability to be manufactured as small devices and at a low cost. A typical magnetoresistive read head is shown in Fig. 2-13.

Fig. 2-13. A magnetoresistive read head. [13]

This figure shows a magnetoresistive device surrounded by a shield. The shield is used to block the surrounding magnetic fields in order to increase the resolution and decrease noise of the read head. This read head scans over the surface of the magnetically recorded medium, the disk, and the magnetic field from the disk interacts with the read head causing an increase or decrease in the resistance of the device. This information gets sent to a computer where it is converted into meaningful data.

The magnetic tunnel junction has many important properties such as the change in the resistance for applied magnetic field strengths and the decrease in resistance for an applied voltage. These properties can be exploited with various applications such as the magnetic field sensor, magnetic memory applications, and the magnetic disk drive read head. It should be noted that the tunneling resistance decreases with increasing temperature, which can be unfavorable for some applications.

CHAPTER 3. FIRST PRINCIPLES FOR THEORETICAL MODELING

A theoretical model for the behavior of magnetic tunnel junctions will be derived from first principles including the density of states, tunneling probability, magnetic effects, and the number of charge carriers. From these basic principles the current density, resistance area product, and the magnetoresistance for a magnetic tunnel junction will be formulated. A detailed discussion of the derivation of the density of states for a free electron "open" electronic band as well as a closed band and the WKB (Wentzel, Kramers, Brillouin) approximation for the probability of tunneling is included to give the development of the tunneling junction model a more complete form. This derivation was based on the density of states of an open band results of Livingston [14] and the tunneling probability results of Griffiths [15]. The magnetic tunnel junction band structure for the parallel and antiparallel magnetization configurations used for this thought process is that in Fig. 2-3 and the physical structure of this tunnel junction is that shown in Fig. 2-9.

Density of States

Two methods for defining the density of states for the band structure of the two electrodes in the magnetic tunnel junction were investigated. The first function used to describe the density of states was the free electron model, which is widely used in condensed matter physics to describe electron states in metals. Under these assumptions the density of states $D(E)$ varies with the square root of the energy for an open band structure. Later a second function was used in order provide electron energy bands of finite width. The second function varies with a polynomial function of the energy and gives a finite width closed band structure. In this case a

second order function was found which gave exact analytical results. The emergence of an exact analytic solution in the case of the finite band was considered to be an important result.

DENSITY OF STATES FOR A FREE ELECTRON "OPEN" BAND

A free electron open band structure is a band structure where electrons are allowed to continuously fill the band and there are no forbidden energies. Starting with the three dimensional time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi + V(x,y,z)\psi = E\psi$$

where $V(x,y,z)$ is the potential energy and can be given by what is called the "particle in a box" approach. This can be represented by a box where inside the box the potential $V(x)$ is zero and outside the box the potential $V(x)$ is infinite. This completely constrains the electron to lie in the box, although within the box the electron has no constraints, and is therefore "free" within this limitation. For conceptual purposes it is often assumed that the boundaries of the potential energy well are the macroscopic boundaries of the material, and this gives rise to a set of allowed energy states for the electrons. A more mathematical definition of this potential energy function is given below

$$V(x,y,z) = \begin{cases} 0, & \text{if } 0 \leq x \leq L, 0 \leq y \leq L, 0 \leq z \leq L, \\ \infty, & \text{otherwise} \end{cases}.$$

When the potential energy is zero and by using the method of separation of variables the Schrödinger equation can be simplified into three separate equations for each Cartesian axis

$$\frac{d^2\psi_x}{dx^2} = -k_x^2\psi_x, \text{ and } \frac{d^2\psi_y}{dy^2} = -k_y^2\psi_y, \text{ and } \frac{d^2\psi_z}{dz^2} = -k_z^2\psi_z$$

where the total energy, E , is given by $E = E_x + E_y + E_z$ and each k is defined as

$$k_x = \frac{\sqrt{2m_e E_x}}{\hbar}, \text{ and } k_y = \frac{\sqrt{2m_e E_y}}{\hbar}, \text{ and } k_z = \frac{\sqrt{2m_e E_z}}{\hbar}.$$

Applying the boundary conditions the solutions to these equations are

$$\psi_x = A_x \sin(k_x x), \text{ and } \psi_y = A_y \sin(k_y y), \text{ and } \psi_z = A_z \sin(k_z z)$$

where each k is found to take discrete values according to the following equations where all n values are integers ranging from 1 to ∞

$$k_x = \frac{n_x \pi}{L}, \text{ and } k_y = \frac{n_y \pi}{L}, \text{ and } k_z = \frac{n_z \pi}{L}.$$

The allowable energy levels are given by the following where $k = k_x + k_y + k_z$

$$E = \frac{\hbar^2 k^2}{2m_e}.$$

Plotting the possible values of k forms a positive, three-dimensional “k-space” in which each point is separated by π / L giving a volume for each “k-space” block of π^3 / L^3 which is equivalent to the volume of one state. When this space is filled with electrons each volume element is allowed to contain at most two electrons due to the Pauli Exclusion Principle.

However, the magnetic tunnel junction model that has been developed here will treat each electron state (either spin up or spin down) separately and this will only allow one electron of each type in this volume element, thereby filling N_s states.

There can be more than one state with the same energy (i.e. degenerate states). The values for n_x , n_y , and n_z that give the same energy all lie along a vector k. The volume contained in a radius k of k-space is given by

$$\frac{1}{8} \left(\frac{4}{3} \pi k^3 \right).$$

The number of states contained in this volume is

$$N_s = \frac{L^3 k^3}{6\pi^2}.$$

When the k relation to the energy is substituted into the above equation the number of states given up to an energy E is found to be

$$N_s(E) = \frac{L^3}{6\pi^2 \hbar^3} (2m_e E)^{3/2}.$$

The number of states in each energy interval (or density of states) is found from the derivative of the above function

$$D(E) = \frac{L^3 m_e}{2\pi^2 \hbar^3} \sqrt{2m_e E}.$$

From this function the density of states continuously increases with increasing energy. The density of states will always be denoted as $D(E)$.

DENSITY OF STATES FOR A CLOSED BAND

The closed band structure for the density of states gives a more realistic description of how the density of states varies with increasing energy in a real material. This type of behavior is most evident in materials where the band becomes filled, or nearly filled, with electrons. This means that there are certain energy values for which no electron state is allowed, and within the confines of the model described below we assume that above a certain energy level no electron states will be found, so called “forbidden” energies. This approximation is realistic if there are no electrons at higher energy levels, because if the energy states are not occupied, the material will behave in the same way as if there were simply no energy states present.

This is not difficult to model with a finite bandwidth model, while still using Fermi-Dirac statistics. Metals have this type of band structure; however, the conduction band in a metal is not totally filled with electrons. Therefore a partially filled finite electron band is used as the next nearest approximation (after the free electron model) to a real material.

In this case the density of states for a “closed” or finite band can be modeled using a parabola which intersects the energy axis at two points. The equation for the density of states for a closed parabolic band of this type has the form of

$$D(E) = \left(\frac{D_1}{E_1^2 - E_1 E_2} \right) E^2 - \left(\frac{E_2 D_1}{E_1^2 - E_1 E_2} \right) E$$

where E_1 , D_1 , and E_2 are all constants which can be used to parameterize the shape of the band. A plot of this function is shown in Fig. 3-1.

Fig. 3-1. Closed parabolic band structure showing constants D_1 , E_1 , and E_2 .

Values for the above constants were chosen to agree broadly with the values for the density of states for the open band structure. Therefore, D_1 will be on the order of 10^{22} (the order of

magnitude found using the free electron density of states), and E_2 will be greater than the Fermi energy of the material because the electrodes are metals and E_1 will be somewhere in between E_2 and the Fermi level. The above two equation for the density of states holds for spin up as well as for spin down electrons. It should be noted that for a metallic material the Fermi level could be located anywhere within the band in the closed band structure, however to ensure a simplified model the energies will be defined as in Fig. 3-1 and in the above discussion.

Although real band structures are finite, they do not usually follow such a smooth curve. The density of states for FeCo is shown in Fig. 3-2.

Fig. 3-2. Density of states for FeCo. [16]

In the above figure it is seen that the bands are shifted due to a magnetic exchange energy which is discussed below. Near the Fermi energy it is seen that the density of states follows a structure approximately like that of the closed electronic band.

Probability of Tunneling

A distinction should be made between the physical barrier and the energy barrier. The physical barrier is the oxide layer of the magnetic tunnel junction and the thickness of this layer is the physical thickness of the oxide. The energy barrier is a barrier seen by the electrons and the thickness of this barrier can be different from the physical thickness of the oxide layer. Since the tunneling barrier in a magnetic tunnel junction does not have sharp, well-defined walls (for example because of diffusion of chemical species at the interfaces), nor does it have a constant energy over its length (meaning the potential energy of the barrier varies as a function of distance), the solution to Schrödinger's equation is therefore more difficult than in the simplified cases of Simmons and Brinkman. To aid in solving this problem the WKB approximation will be used.

To begin, the one-dimensional time-independent Schrödinger equation is given as

$$-\frac{\hbar^2}{2m_e} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

this equation can be simplified to

$$\frac{d^2\psi}{dx^2} = -\kappa^2\psi$$

where κ is defined as

$$\kappa(x) = \frac{\sqrt{2m_e (E - V(x))}}{\hbar}$$

The region of concern for this tunneling model is within the barrier, therefore, κ will be imaginary since all of the energies that are involved in the tunneling process will be less than

the potential energy of the barrier ($E < V(x)$). The general solution to the simplified, one-dimensional, time-independent Schrödinger equation above is:

$$\psi(x) = A(x)e^{\phi(x)}$$

where $A(x)$ and $\phi(x)$ are defined as the amplitude and the phase respectively. When the potential energy varies as a function of distance the amplitude and the phase of the wavefunction may also vary with distance.

The general solution must be used in the simplified one-dimensional, time-independent Schrödinger equation to solve for $A(x)$ and $\phi(x)$. The first and second derivatives of the general solution function are found to be

$$\frac{d\psi}{dx} = (A' + A\phi')e^{\phi} \quad \text{and} \quad \frac{d^2\psi}{dx^2} = [A'' + 2A'\phi' + A\phi'' + A(\phi')^2]e^{\phi}.$$

When these equations are substituted into Schrödinger's equation they give

$$A'' + 2A'\phi' + A\phi'' + A(\phi')^2 = -\kappa^2 A$$

multiplying both sides by A the above equation can be simplified to

$$(A^2\phi')' + (A\phi')^2 = -\kappa^2 A^2$$

for the WKB approximation to work it is assumed that the amplitude varies slowly with distance making the second derivative of A negligible. It was stated earlier that κ is imaginary, therefore, the phase $\phi(x)$ must also be imaginary. The squares of κ and ϕ will yield real numbers while their derivatives will yield imaginary numbers. This allows Schrödinger's equation to be broken up into two parts a real part and an imaginary part:

$$\text{Real: } (\phi')^2 = \kappa^2$$

$$\text{Imaginary: } (A^2\phi')' = 0$$

These two parts can be solved individually, as shown below. For the imaginary part

$$A = \frac{C}{\sqrt{|\phi'|}}$$

where C is a real constant and from the real part

$$\phi(x) = \pm \int |\kappa(x)| dx.$$

Putting these together gives the tunneling wavefunction

$$\psi(x) \cong \frac{C}{\sqrt{|\kappa(x)|}} e^{\pm \int |\kappa(x)| dx}.$$

For a barrier with a varying potential there will be three separate regions: region I has $E > V(x)$, region II has $E < V(x)$, and region III is similar to region I with $E > V(x)$. A diagram of this potential energy "surface" is illustrated in Fig. 3-3.

Fig. 3-3. Potential energy "surface" for an energy barrier. [15]

For regions I and III the solutions to Schrödinger's equations are the same

$$\psi(x) = (\text{Constant})e^{ikx} \text{ or } \psi(x) = (\text{Constant})e^{-ikx}$$

where the positive exponential term indicates a wave traveling in the positive x direction and the negative exponential term indicates a wave traveling in the negative x direction and k is given by

$$k = \frac{\sqrt{2m_e E}}{\hbar}$$

because in these two regions the potential energy is zero. The solution in region I consists of two waves, one incident wave and one reflected wave, therefore the wavefunction for this region will be a linear combination of these two waves with incident amplitude of A and reflected amplitude of B.

Region I,

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

Region III consists of only one transmitted wave with a transmitted amplitude of F.

Region III,

$$\psi(x) = Fe^{ikx}$$

Region II consists of two exponential functions an increasing exponential with amplitude of C and a decreasing exponential with amplitude of D. From the results given above for the wavefunction within the barrier the total wavefunction is written as a linear combination of the increasing, C, term and the decreasing, D, term.

$$\psi(x) = \frac{C}{\sqrt{|\kappa(x)|}} e^{\int_0^x |\kappa(x)| dx} + \frac{D}{\sqrt{|\kappa(x)|}} e^{-\int_0^x |\kappa(x)| dx}$$

If the barrier has a large potential energy compared to the energy of the tunneling wave or the barrier is sufficiently thick the C term will go to zero.

Region II,

$$\psi(x) = \frac{D}{\sqrt{|\kappa(x)|}} e^{-\int_0^x |\kappa(x)| dx}$$

The tunneling probability (also known as the transmission coefficient) is given by

$$T = \frac{|F|^2}{|A|^2}$$

which is the fraction resulting from the electrons found in region III and the electrons incident in region I. The amplitude of the incident wavefunction decreases exponentially from A to F in region II. At $x = a$ it is found that

$$F = A \frac{D}{\sqrt{|\kappa(x)|}} \text{Exp} \left[-\int_0^a |\kappa(x)| dx \right].$$

Therefore, the tunneling probability is given by

$$T \cong \text{Exp}[-2 \int_0^a |\kappa(x)| dx].$$

From this point the tunneling probability will be labeled as $P(E)$ instead of T . When this tunneling probability is used for modeling the potential energy, $V(x)$, is usually approximated by $V(x) = E_F + \phi(x)$ where E_F is the Fermi energy and $\phi(x)$ is the height of the barrier as a function of distance. By substituting this equation for the potential energy and the equation for kappa, the tunneling probability for an electron with energy E is then described by

$$P(E) = \text{Exp} \left[-\frac{2}{\hbar} \int_0^a \sqrt{2m_e (E_F + \phi(x) - E)} dx \right].$$

It can be shown [6] that the integral in the above exponential function can be approximated by

$$P(E) = \text{Exp}[-A \sqrt{E_F + \bar{\varphi} - E}]$$

where $\bar{\varphi}$ is the average barrier height of the tunneling barrier and A is defined as

$$A = \frac{2\beta a \sqrt{2m_e}}{\hbar}$$

where β is a factor that arises from the approximation and can usually be taken to be unity (for an explanation see [6]). A tunnel junction is usually modeled by assuming that the average barrier height takes a trapezoidal shape when a voltage is applied to the tunnel junction.

According to the Brinkman model the average barrier height is then defined as

$$\bar{\varphi} = \varphi - eV / 2$$

where φ is the initial barrier height before the voltage is applied.

These assumptions lead to the final simplified form of the tunneling probability

$$P(E) = \text{Exp}[-A \sqrt{E_F + \varphi - \frac{eV}{2} - E}].$$

It should be noted that the shape of the potential energy barrier is most likely not perfectly trapezoidal; other shapes of the barrier such as the inclusion of image forces [6] will not be discussed in this thesis. Image forces are forces experienced by the electron when it approaches the energy barrier. For simplicity these forces will not be discussed in this study.

Magnetic Effects

There are two different types of magnetic effects that could occur within the magnetic tunnel junction, these are 1) an applied magnetic field that is strong enough to cause a change in the electronic band structure of the magnetic layers and 2) an applied magnetic field that is weaker but will cause a reversal of the orientations of the magnetizations of the magnetic layers. The

first effect takes a large amount of energy because the electron spins are "coupled" to each other due to a magnetic exchange interaction energy. If a magnetic field is applied to the device at this field strength the number of electrons in both the spin up states and the spin down states will change to result in a net magnetic moment which is aligned with the applied magnetic field. This exchange energy causes one electron state (either spin up or spin down) to shift its density of states function downwards and the other electron state to shift its density of states function upwards. Experimental data suggests that there is a different mechanism that causes the orientations of the magnetic layers to change because the magnetic fields that are needed are much smaller than the fields needed to overcome the exchange interaction energy. To model this, it will be assumed that the electrons are only allowed to be either aligned parallel or antiparallel to the applied magnetic field. This will give only two results a high resistance or a low resistance. The basic theory for the magnetization of single-electron atoms in a magnetic field will be used as an analogy to the parallel and antiparallel orientations of the tunnel junction.

First, consider a group of single-electron atoms (for simplicity it will be assumed that only one electron per atom will be involved in the magnetic effects of the electrode in a magnetic tunnel junction). If a magnetic field, H , is applied to this group of single-electron atoms only two states are possible for each electron; the electron can be aligned either parallel (spin up) or antiparallel (spin down) to the applied magnetic field. The magneto-static energy of a magnetic moment in an applied magnetic field is given by

$$E = -\mu_0 \vec{m} \cdot \vec{H}$$

here m is the magnetic moment and μ_0 is the permeability of free space. When discussing magnetic effects m will always be the moment and μ will always be the permeability. The probability of finding an electron in one of the two states follows the Fermi – Dirac statistics, however for very large E the following equation for the probability may be used

$$P_n = C \text{Exp} \left[\frac{-E_n}{kT} \right].$$

This allows the probability of occupancy of each state to be written as

$$P_{up} = C \text{Exp} \left[\frac{+\mu_0 m H}{kT} \right] \text{ and } P_{down} = C \text{Exp} \left[\frac{-\mu_0 m H}{kT} \right].$$

Since these are the only two possible states for the magnetic moment of the electron in the applied magnetic field the constant C is found to be

$$C = \frac{1}{\text{Exp} \left[\frac{+\mu_0 m H}{kT} \right] + \text{Exp} \left[\frac{-\mu_0 m H}{kT} \right]}$$

from the fact that

$$P_{up} + P_{down} = 1$$

because the probability of finding the electron in either a spin up or a spin down state is 100 percent. The total magnetization of the material is found by the difference between the parallel and antiparallel configurations giving

$$M = N m_{electron} (P_{up} - P_{down}) = N m_{electron} \tanh \left(\frac{\mu_0 m_{electron} H}{kT} \right).$$

M will always be positive because the positive exponent in P_{up} will always be greater than the negative exponent in P_{down} . In the above equation the electronic magnetic moment, $m_{electron}$,

should not be confused with the mass of the electron, m_e . From this equation the total magnetic moment of the material may be found by

$$m_{total} = m_{electron} \tanh\left(\frac{\mu_0 m_{electron} H}{kT}\right)$$

where $m_{electron}$ is the magnetic moment of one electron or one Bohr magneton, μ_b . This gives the total external energy of a material in an applied magnetic field as

$$E_{app} = -\mu_0 \vec{m}_{Total} \cdot \vec{H}.$$

The energy due to the magnitude of the applied magnetic field will be much less than the energy due to the coupling of the electronic spins in a magnetic material used in a magnetic tunnel junction. For this reason the applied magnetic field will not significantly change the band structure of the metallic electrodes, but will only change the orientation of the two electrodes with respect to each other.

It should be noted, for the purpose of completeness, that most magnetic materials involve atoms in which more than one electron contributes to the magnetic properties and will therefore follow a slightly different equation for the magnetization of the material. [17] The magnetization is found by

$$M = NmB_J \left[\frac{\mu_0 m (H + \alpha M)}{kT} \right]$$

where $B_J(x)$ is the Brillouin function given by

$$B_J(x) = \left(\frac{(2J_q + 1)}{2J_q} \right) \coth \left(\frac{(2J_q + 1)x}{2J_q} \right) - \left(\frac{1}{2J_q} \right) \coth \left(\frac{x}{2J_q} \right)$$

and J_q is the total quantum angular momentum not to be confused with the current density.

This equation is given without proof here and will not be used in the calculations for the theoretical model in order to maintain a simplified model.

For a magnetic tunnel junction the result for the magnetic field on the band structure above may be used in a similar analogy by substituting the resistance instead of the magnetization.

The tunnel junction has only two possible configurations parallel and antiparallel.

Assuming that the tunnel junction as a whole can be considered to have magnetic orientations in either of two configurations, parallel or antiparallel, the applied magnetic field will follow the same type of behavior outlined in the above discussion on the magnetic effects in relation to the band structure. To model this behavior the equation should have two sets of hyperbolic functions, one describing the applied magnetic field affecting the first electrode and one describing the applied magnetic field affecting the second electrode. For a low magnetic field (which in this case includes negative fields) the tunnel junction should begin in the parallel configuration and upon increasing the magnetic field the tunnel junction will switch to the antiparallel configuration. This assumes that previously a large magnetic field has been applied in the negative direction to the tunnel junction and then dropped back to zero. If the magnetic field is further increased the tunnel junction returns to the parallel configuration due to the changing in the direction of the magnetic moment of the antiferromagnetically "pinned" layer.

An equation was needed that demonstrates the above behavior of the resistance versus the applied magnetic field. It is assumed that the tunnel junction can only be in one of two orientations, either parallel or antiparallel. Using this idea the hyperbolic tangent function

would describe this transition well. However, this function alone does not describe the transition back to the parallel orientation. This hyperbolic function can be shifted along the x axis to any point, therefore if two hyperbolic functions were used in an equation it would describe a shape similar to that of the experimental results of the resistance versus the applied magnetic field. As a first approximation this equation is assumed to take the following form

$$R(x) = (A \tanh(x - a) + B) \tanh(x - b) + C$$

where b is greater than a . As x goes to negative infinity the value of $R(x)$ should be equal to the resistance of the parallel orientation. If x is between a and b then the value of $R(x)$ should be equal to the resistance of the antiparallel orientation. As x goes to positive infinity the value of $R(x)$ should again be equal to the resistance of the parallel orientation. These statements can be expressed symbolically as

$$\begin{aligned} x \rightarrow -\infty : A - B + C &= R_{\text{parallel}} \\ (a < x < b) : -A - B + C &= R_{\text{antiparallel}} \\ x \rightarrow +\infty : A + B + C &= R_{\text{parallel}} \end{aligned}$$

Solving for A , B , and C gives

$$\begin{aligned} A &= \frac{R_{\text{parallel}} - R_{\text{antiparallel}}}{2} \\ B &= 0 \\ C &= \frac{R_{\text{parallel}} + R_{\text{antiparallel}}}{2} \end{aligned}$$

The values of a and b can be considered to be the coercivities of the free layer and the pinned layer in the magnetic tunnel junction.

With this in mind, the resistance as a function of the applied magnetic field may be written in the following form

$$R(H) = \left(\left(\frac{R_{parallel} - R_{antiparallel}}{2} \right) \tanh \left(\frac{\mu_0 m_1 (H - H_{c1})}{kT} \right) \right) \tanh \left(\frac{\mu_0 m_2 (H - H_{c2})}{kT} \right) + \left(\frac{R_{parallel} + R_{antiparallel}}{2} \right)$$

Where, in the above equation, m_1 and m_2 correspond to the total magnetic moments of electrode one and electrode two respectively; H_{c1} and H_{c2} are the values of the magnetic fields where the tunnel junction switches from parallel to antiparallel, H_{c1} , and back again, H_{c2} . Usually, $H_{c2} > H_{c1}$.

Number of Charge Carriers

The number of charge carriers that travel across the barrier of a magnetic tunnel junction from one electrode to another can be found by finding the number of electrons at each energy level and multiplying that by the probability of tunneling at each energy level; integrating this over all energies up to a finite energy E gives the total number of electrons that tunnel through the barrier. This can be expressed as

$$N = \int D(E) f(E) P(E) dE$$

where $f(E)$ is a function known as the Fermi – Dirac function, $D(E)$ is the density of available states, and $P(E)$ is the probability of tunneling. The Fermi - Dirac equation gives the probability of finding an electron in a band at a certain energy level with varying temperature. This equation is defined as

$$f(E) = \frac{1}{1 + \text{Exp} \left[\frac{E - E_F}{kT} \right]}$$

which at $T = 0$ gives a probability of occupancy of one when $E < E_F$ and a probability of occupancy of zero when $E > E_F$.

When considering tunneling from an electrode with a certain band structure, to another electrode with a certain band structure the probability of finding an empty state in the second electrode for that electron must be taken into account. This is an important consideration because the result is that the density of states in the final electrode affects the number of electrons that are able to tunnel through. The calculation of this effect is accomplished with the following equation

$$N = \iint [(D_1(E)f_1(E)) - (D_2(E)f_2(E))] P(E) dE$$

where the number of electrons in the second electrode at the same energy are subtracted from the number of tunneling electrons from the first electrode which ensures that the electron tunneling is affected by the number of available electron states in either electrode.

This equation will be used for the spin up electrons as well as for the spin down electrons.

The spin up and spin down equations are added together to give the total number of tunneling electrons in the magnetic tunnel junction for either a parallel or an antiparallel magnetization configuration. The number of charge carriers that tunnel for a parallel magnetization configuration is given by

$$N_{parallel} = \int \left\{ \left[(D_1(E + E_{app})f_1(E)) - (D_2(E + E_{app} + eV)f_2(E + eV)) \right] + \left[(D_1(E - E_{app})f_1(E)) - (D_2(E - E_{app} + eV)f_2(E + eV)) \right] \right\} P(E) dE$$

and the number of charge carriers that tunnel for an antiparallel magnetization configuration is given by

$$N_{\text{antiparallel}} = \int \left\{ \left[\left(D_1(E + E_{\text{app}}) f_1(E) \right) - \left(D_2(E - E_{\text{app}} + eV) f_2(E + eV) \right) \right] + \left[\left(D_1(E - E_{\text{app}}) f_1(E) \right) - \left(D_2(E + E_{\text{app}} + eV) f_2(E + eV) \right) \right] \right\} P(E) dE.$$

In the above equations, the ferromagnetic exchange energy can be included into the equation via E_{app} .

Current Density, Resistance Area Product, and Magnetoresistance

Using the above results of the number of charge carriers that tunnel for the parallel and antiparallel magnetization configurations, the current density, resistance area product, and the magnetoresistance may be determined. A few assumptions should be made when applying the derived equations for the number of charge carriers to a model for the current – voltage characteristics. For the purposes for this thesis the tunnel junction has been taken as a whole entity. A voltage will be applied across the electrodes of the magnetic tunnel junction. The current passes through the insulating barrier and exits the junction through the second magnetic electrode. Using this simplifying idea it is assumed that the resistances which are measured in the magnetic tunnel junction are averaged values which result from the device as a whole instead of attempting to pinpoint where within the magnetic tunnel junction these resistances are derived. According to the Drude theory for free electrons, the conductivity of a metal is given as

$$\sigma = \frac{Ne^2\tau}{m_e}$$

where N is the total number of charge carriers for both spin up and spin down electrons, e is the principal charge, τ is the relaxation time, and m is the mass of an electron. Ohm's Law gives a relation between the electric field and the current density

$$J = \sigma E = \sigma \frac{V}{x}$$

where x is the total distance across the tunnel junction and V is the applied voltage. The magnetic tunnel junction is essentially a non-Ohmic device, therefore for the above equation to be valid the conductivity must vary for the two different magnetization orientations of the magnetic tunnel junction. This can be described using a generalized form of Ohm's law.

When the equation for the number of charge carriers is substituted into this equation the ideal result (assuming that the density of states for electrode 1 is always larger than the density of states for electrode 2) is

$$J = \frac{e^2 \tau V}{m_e x} \left(\int [D_{1\uparrow}(E)f_{1\uparrow}(E) - D_{2\uparrow}(E)f_{2\uparrow}(E)] P(E) dx + \int [D_{1\downarrow}(E)f_{1\downarrow}(E) - D_{2\downarrow}(E)f_{2\downarrow}(E)] P(E) dx \right)$$

where the summation takes into account the tunneling of both spin up and spin down electrons across the barrier, and the differences allowed for electrons passing in both directions. This can give the current density as a function of the applied voltage and the applied magnetic field.

If a magnetic field is not applied and there is no ferromagnetic exchange coupling in the electrodes the second integral will be equal to the first. It is then necessary to consider the current density due to tunneling of electrons when either in the parallel or antiparallel magnetization configurations. The equation for the current density of a junction with a parallel configuration of the magnetizations of the electrodes and an applied voltage is

$$J_{parallel} = \frac{e^2 \tau V}{m_e x} \left(\int [(D_{1\uparrow}(E + E_{app})f_{1\uparrow}(E) - D_{2\uparrow}(E + E_{app} + eV)f_{2\uparrow}(E + eV))] P(E) dx + \int [D_{1\downarrow}(E - E_{app})f_{1\downarrow}(E) - D_{2\downarrow}(E - E_{app} + eV)f_{2\downarrow}(E + eV)] P(E) dx \right)$$

where E_{app} is the energy causing the asymmetric nature of the electronic spins in the material (i.e. the exchange energy). The equation for the antiparallel magnetization configuration is given by

$$J_{antiparallel} = \frac{e^2 \tau V}{m_e x} \left(\int \left[(D_{1\uparrow}(E + E_{app})f_{1\uparrow}(E) - D_{2\uparrow}(E - E_{app} + eV)f_{2\uparrow}(E + eV)) \right] P(E) dx \right. \\ \left. + \int \left[(D_{1\downarrow}(E - E_{app})f_{1\downarrow}(E) - D_{2\downarrow}(E + E_{app} + eV)f_{2\downarrow}(E + eV)) \right] P(E) dx \right)$$

Once the general equations for the current density are found the resistance area product is determined using another variation of Ohm's Law

$$R * A = \frac{V}{J}.$$

The resulting equations for the parallel and the antiparallel magnetization configurations are:

$$R * A_{parallel} = \frac{m_e x}{e^2 \tau} \left[\int \left\{ \left[(D_1(E + E_{app})f_1(E)) - (D_2(E + E_{app} + eV)f_2(E + eV)) \right] \right. \right. \\ \left. \left. + \left[(D_1(E - E_{app})f_1(E)) - (D_2(E - E_{app} + eV)f_2(E + eV)) \right] \right\} P(E) dE \right]^{-1}$$

$$R * A_{antiparallel} = \frac{m_e x}{e^2 \tau} \left[\int \left\{ \left[(D_1(E + E_{app})f_1(E)) - (D_2(E - E_{app} + eV)f_2(E + eV)) \right] \right. \right. \\ \left. \left. + \left[(D_1(E - E_{app})f_1(E)) - (D_2(E + E_{app} + eV)f_2(E + eV)) \right] \right\} P(E) dE \right]^{-1}$$

To complete the formulation of the major properties of the magnetic tunnel junction, i.e. voltage and magnetic effects on the resistance, the above two equations are used in the equation for the resistance area product as a function of the applied magnetic field

$$R * A(H) = \left(\left(\frac{R * A_{parallel} - R * A_{antiparallel}}{2} \right) \tanh \left(\frac{\mu_0 m_1 (H - H_{c1})}{kT} \right) \right) \tanh \left(\frac{\mu_0 m_2 (H - H_{c2})}{kT} \right) \\ + \left(\frac{R * A_{parallel} + R * A_{antiparallel}}{2} \right)$$

The magnetoresistance is a way of characterizing a magnetic tunnel junction. The magnetoresistance is defined as

$$\frac{\Delta R}{R} = \frac{R_{\text{antiparallel}} - R_{\text{parallel}}}{R_{\text{parallel}}}$$

Inserting the equations of the resistance area product into the above equation for the magnetoresistance and canceling common values gives

$$\frac{\Delta R}{R} = \frac{\tau_{\text{parallel}}}{\tau_{\text{antiparallel}}} \frac{N_{\text{parallel}}}{N_{\text{antiparallel}}} - 1$$

where N_{parallel} refers to the net number of electrons tunneling through the barrier when the magnetizations are parallel, $N_{\text{antiparallel}}$ refers to the net number of electrons tunneling through the barrier when the magnetizations are antiparallel, and τ_{parallel} and $\tau_{\text{antiparallel}}$ are the relaxation time constants for the parallel and antiparallel orientations. This equation depends upon the ratio of the number of charge carriers in the two configurations and also the ratio between the two relaxation time constants. The physical dimensions of the tunnel junction as well as values such as the relaxation time constant are not needed. At absolute zero of temperature the magnetoresistance equation above may be solved analytically; this expanded equation for the magnetoresistance is shown in the Appendix.

When a magnetic field is applied in the opposite direction to the magnetization in the two electrodes while in their parallel configuration, the magnetization of the tunnel junction can be changed from a parallel configuration to an antiparallel magnetization configuration by reorienting the free layer, and hence the resistance can be increased. If the magnetic field is increased beyond the switching field of the antiparallel configuration the tunnel junction

changes back to a parallel magnetization configuration, with both layers having their magnetization along the field direction, and the resistance will again decrease.

This chapter has presented the basic formulas including the current density, resistance area product and the magnetic field effects of the new theoretical model for magnetic tunnel junctions. The next chapter will go into detail about the application of this model to experimental data.

CHAPTER 4. RESULTS AND DISCUSSION

In the previous chapter the basic principals of the new theoretical model for magnetic tunnel junctions were introduced. In this chapter they will be expanded, solutions to the equations will be calculated and the model will be applied to actual experimental data. The new theoretical model will then be compared to earlier models such as the Simmons model.

Resulting Band Structures

The number of electrons at a given energy level is given by the following equation

$$N(E) = D(E)f(E)$$

which is the density of states multiplied by the probability of occupancy (the Fermi – Dirac statistics).

The typical parabolic model for a non-magnetic band structure of an ideal free electron metal is shown in Fig. 4-1.

Fig. 4-1. Parabolic model of a non-magnetic band structure of a free electron metal.

This figure shows that as more electrons are added the ground state energy must increase; half of these states will contain electrons with spin up and the other half will be spin down. In a

magnetic material the band structure changes and the electronic spins attempt to align with the magnetic field and this gives one spin direction a lower energy and increases the number of these electrons. This causes the band structure of the material to change from Fig. 4-1 to that of Fig. 4-2.

Fig. 4-2. Parabolic model of the band structure in a free electron magnetic material showing the exchange splitting of the energy states.

The shift in the energy of the spin up and spin down states of the band structure is governed by the exchange interaction. The total magnetic moment per atom in this case results from the difference in occupancy of states for the spin up and spin down electrons.

If a voltage is applied across a tunnel junction the electron bands of the electrodes will also change in energy. The result will be that the entire band will be shifted up or down by an amount of energy eV . This study will only be concerned with the downward shift of the band structure with a positive applied voltage.

When these concepts are combined and introduced for the metallic electrodes of the magnetic tunnel junction the band structure of the junction with parallel magnetization configuration will look similar to Fig. 4-3.

Fig. 4-3. Parallel magnetization alignment of the two electrodes with a parabolic band structure for a magnetic tunnel junction.

The band structure corresponding to antiparallel magnetization configuration of the electrodes is shown in Fig. 4-4.

Fig. 4-4. Antiparallel magnetization alignment of the two electrodes with a parabolic band structure for a magnetic tunnel junction.

In figures 4-3 and 4-4, because of limitations on the change of spin polarization, the electrons are only allowed to tunnel into states which have the same spin orientation as those that an electron currently occupies (i.e. a spin up electron tunnels into a spin up state, but not a spin down state). As an example, let the left sides of each band represent the spin down electrons and the right sides of each band represent the spin up electrons. It can be seen from Fig. 4-3 that the two density of states curves are similar, but shifted down by an amount eV . In Fig. 4-3 the number of states available at a given energy for an electron to tunnel into the final

electrode is large. On the other hand, from Fig. 4-4, it can be seen that the majority electrons in the electrode of origin have far fewer states to tunnel into in the final electrode. The end result of this is that there is a higher resistance in the antiparallel magnetization configuration than in the parallel magnetization configuration.

To better illustrate which electrons are involved in the tunneling process the band structure for the two electrodes will be plotted by overlapping each other; the number of available electrons for tunneling will be plotted also. An example of a parallel magnetization configuration is shown in Fig. 4-5. This shows the band structure for electrode 1 (electrode of origin), shown as the band with the higher Fermi energy in black, and the band structure for electrode 2 (final electrode), shown as the band with the lower Fermi energy in green. The number of available tunneling electrons in electrode 1 is shown in red.

Fig. 4-5. Band structure for parallel magnetization of the two electrodes. Black – electrode 1, Green – electrode 2, Red – number of tunneling electrons.

The antiparallel configuration is somewhat more difficult to visualize. One spin orientation may be treated the same as that for the parallel case, however the other spin orientation does not calculate as easily. Fig. 4-6 shows the band structure of the electrodes and the resulting tunneling charge carriers for the antiparallel case.

Fig. 4-6. Band structure for the antiparallel magnetization of the two electrodes. Black – electrode 1, Green – electrode 2, Red – number of tunneling electrons.

From Fig. 4-6 it can be seen that one side of the band structure for electrode 1 contains more available tunneling electrons than the number of available states in electrode 2. To find the number of available tunneling electrons when this occurs the band in electrode 2 needs to be extended to the Fermi level in electrode 1 and that function will be subtracted from the original density of states function for that spin state in electrode 2. This can be better understood as an equation such as

$$N_{\uparrow\text{or}\downarrow}(E) = (D_2 f_1(E) - D_2 f_2(E))_{\uparrow\text{or}\downarrow}$$

where the arrows indicate that, as far as the electrical current is concerned the electrons tunneling could be either spin up or spin down electrons. The result of this calculation is

shown in red on the right hand side of Fig. 4-6. It should be noted that this modification of the equation for the number of charge carriers is only valid for the antiparallel magnetization configuration of the magnetic tunnel junction. The probability term in the equation giving the number of charge carriers reduces the total number of available electrons from the above to the number of electrodes that actually tunnel through the barrier.

The band structure at the Fermi energy and at room temperature does not change appreciably from the band structure at absolute zero temperature, and therefore calculations made nominally at 0 K can be used as a guide to the behavior at ambient temperatures. Using this fact the equation for the magnetoresistance can be expressed as

$$\frac{\Delta R}{R} = \frac{\int_{E_F - eV}^{E_F} D_{\uparrow 1}(E + E_{app1})P(E)dx + \int_{E_F - eV}^{E_F} D_{\downarrow 1}(E - E_{app1})P(E)dx}{\int_{E_F - eV}^{E_F} D_{\downarrow 1}(E - E_{app1})P(E)dx + \int_{E_F - eV}^{E_F} D_{\downarrow 2}(E - E_{app2} + eV)P(E)dx} - 1$$

where the second term in the denominator includes the correction for the number of tunneling electrons in the antiparallel configuration, as discussed above. Here the E_{app} terms are the energy of the ferromagnetic exchange coupling in the band structure for each electrode. This is due to the fact that the energy due to the applied magnetic field is so small compared to this coupling energy that the coupling energy is the most dominate and therefore is used as E_{app} . The results of this section were calculated from a free electron density of states, however, the results may be easily found for a finite width band structure.

Fitting the Model to Data and Adjustments to the Model

Magnetoresistance data were gathered from a magnetic tunnel junction supplied by

Nonvolatile Electronics, Inc using a probe station designed to apply a voltage to an individual

tunnel junction and by then measuring the resulting resistance. The magnetoresistance probe station used to obtain this data is shown in Fig. 4-7.

Fig. 4-7. Magnetoresistance probe station.

The tunnel junctions that were measured had the following structure: NiFe (120 Å) – AlOx (15 Å) – FeCo (54 Å) – CrPrMn (328 Å) – Al (54 Å). The NiFe layer is a magnetic layer that is weakly coupled to the FeCo magnetic layer. The CrPrMn layer is an antiferromagnetic material which effectively “pins” the FeCo, via exchange coupling, which causes the layer to switch magnetization directions at an applied magnetic field that is higher than its normal switching field strength in its uncoupled state. The tunneling area for the junction that provided the experimental data had a nominal value of $285 \times 285 \mu\text{m}^2$ and the thickness of the tunnel junction was 57.1 nm. Fig. 4-8 shows the structure that was tested using the magnetoresistance probe station.

Fig. 4-8. Magnetic tunneling junctions tested from Nonvolatile Electronics, Inc.

Fig. 4-8 shows five tunneling junctions. The tunnel junction in the upper right corner is a single tunnel junction and the rest are double tunnel junctions; it is this single junction that was most important. Using the probe station, a magnetic field was applied to the tunnel junction and the resistance was measured. The parallel and antiparallel magnetization configurations were found at the lowest and highest plateau in the resistance versus the applied magnetic field curve. Once the resistances for these two magnetization configurations were determined the magnetoresistance as a function of voltage was calculated. The magnetic field was not applied at sufficient strength to cause a reversal in the magnetization of the FeCo electrode. The results for the tested tunnel junction are found in Figs. 4-9 and 4-10 for the variation of the resistance versus the applied magnetic field and the magnetoresistance versus the applied voltage respectively.

Fig. 4-9. Resistance area product as a function of the applied magnetic field for the tested magnetic tunnel junction.

This figure shows the resistance area product as a function of the applied magnetic field for the magnetic tunnel junction tested from Nonvolatile Electronics, Inc. Fig. 4-10 shows how the magnetoresistance varies as a function of the applied voltage.

Fig. 4-10. Magnetoresistance as a function of the applied voltage for the same magnetic tunnel junction as Fig. 4-9.

The magnetoresistance of this particular tunnel junction was calculated and found to be 25%.

The applied magnetic field for the parallel and antiparallel magnetization configurations was ± 4 Oe, (+ for the antiparallel magnetization configuration and – for the parallel magnetization configuration). The resistance area product as a function of the applied voltage for both the parallel and antiparallel magnetization configurations are shown in Fig. 4-11.

Fig. 4-11. Resistance area product as a function of the applied voltage. Black – antiparallel; Red – parallel.

First the new model was fitted to the experimental data for the current density versus the applied voltage for the parallel magnetization configuration as well as the antiparallel magnetization configuration. The theoretical model appeared to fit the current density data well, however, when the resistance area product was calculated using the generalized Ohm's law the theory deviated from the experimental behavior. This is most likely due to the fact that the quotient of V/J will enhance any differences between the theory and the experimental data for the resistance area product at low voltages especially because both V and J tend toward zero for decreasing voltages. The predicted resistance area product at low voltages can be corrected by using a prefactor. This prefactor is shown in the equation below.

$$RxA = \left(\frac{V + V_1}{V + V_2} \right) \left(\frac{m_e x}{e^2 \tau} \left[\int [D_{1\uparrow}(E)f_{1\uparrow}(E) - D_{2\uparrow}(E)f_{2\uparrow}(E)]P(E)dx \right]^{-1} + \int [D_{1\downarrow}(E)f_{1\downarrow}(E) - D_{2\downarrow}(E)f_{2\downarrow}(E)]P(E)dx \right)^{-1}.$$

The term in front ($mx/e^2\tau$), which will be designated as Q , was allowed to vary during the fitting of the data; this resulted in a different mobility for the parallel and antiparallel magnetization configurations. The density of states function that was used is the equation for the closed band structure was given in chapter 3. A few terms in the equation for the resistance area product were allowed to remain constant for each electrode. The values for these constants for each electrode are shown in Table 4-1.

Table 4-1. Constant values used for the electrode 1 and the electrode 2 band structures.

Electrode 1	Electrode 2
$D_1 = 1.8 \times 10^{22}$	$D_1 = 1.8 \times 10^{22}$
$E_1 = 1 \text{ eV}$	$E_1 = 1 \text{ eV}$
$E_2 = 3 \text{ eV}$	$E_2 = 3 \text{ eV}$
$E_{app} = 0.135 \text{ eV}$	$E_{app} = 0.9 \text{ eV}$

The Fermi energy was defined as reference zero for the tunnel junction. The values for E_{app} in each electrode were found in the two references on the band structures of permalloy and permendur. [16, 18] In these papers the total difference in the energy between the splitting of the band structure was determined and the values which were used for E_{app} were half of the total difference between the energies of each state. The values for E_1 and E_2 were found using an approximation to the band structures of FeCo and NiFe. The value for D_1 was found by solving the free electron density of states for an energy near the fermi level of electrode 1. An illustration of the band structure for electrode 1 (NiFe) is shown in Fig. 4-12.

Fig. 4-12. The band structure used for electrode 1 (NiFe).

An illustration of the band structure for electrode 2 (FeCo) is shown in Fig. 4-13.

Fig. 4-13. The band structure used for electrode 2 (FeCo).

The parameters that were allowed to vary in this fit were Q , s , and ϕ where s and ϕ are the barrier thickness and height respectively and also the voltage parameters V_1 and V_2 were allowed to vary. The values of the parameters found for the parallel magnetization configuration are shown in Table 4-2.

Table 4-2. Values of the parameters for the theoretical model of the parallel magnetization configuration to fit the experimental data.

$Q \text{ (Ohm} \cdot \text{cm}^2) =$	1.65×10^{16}
$s \text{ (Ang)} =$	8.2
$\phi \text{ (eV)} =$	3
$V_1 \text{ (V)} =$	0.002
$V_2 \text{ (V)} =$	3.29

The values of the parameters found for the antiparallel magnetization configuration are shown in Table 4-3.

Table 4-3. Values of the parameters for the theoretical model of the antiparallel magnetization configuration to fit to the experimental data.

$Q \text{ (Ohm} \cdot \text{cm}^2) =$	6×10^{21}
$s \text{ (Ang)} =$	1
$\phi \text{ (eV)} =$	2
$V_1 \text{ (V)} =$	0.002
$V_2 \text{ (V)} =$	3.87

The resulting curves for the theoretical model which uses these parameters are shown with the experimental data for the parallel and antiparallel magnetization configurations in Fig. 4-14.

These parameters were fit to the experimental data by hand and therefore they should not be taken as the only possible values that fit these equations to the experimental data. Therefore there may be values for the antiparallel configuration that result in a barrier thickness parameter that is closer to the physical thickness.

Fig. 4-14. Results of curve fitting. Red – experimental data, Black – model, Triangle – antiparallel, Square – parallel.

Using the value of Q for the parallel and the antiparallel configurations and knowing the values of m , e , and x (which is the thickness of the magnetic tunnel junction), the relaxation time, τ , was determined. This was used to find the mobility of the electrons across the junction for the parallel and antiparallel magnetization configurations. The charge carrier mobility for the parallel configuration was found to be about $2.16 \times 10^{-3} \text{ cm}^2/(\text{V}\cdot\text{s})$ and the charge carrier mobility for the antiparallel configuration was found to be about $5.94 \times 10^{-9} \text{ cm}^2/(\text{V}\cdot\text{s})$. It was expected that the mobility of the electrons for the parallel configuration should be greater than the mobility for the antiparallel configuration due to the lower resistance in the parallel configuration. The values for these mobilities are low compared to the mobilities in a metal which are on the order of $10 \text{ cm}^2/(\text{V}\cdot\text{s})$. The difference is possibly

due to the insulating barrier. However, mobilities closer to this value may be used in the equation, but the number of tunneling electrons must be reduced. The best way to do this would be to increase the barrier height and the thickness.

The resistance area product for the parallel and antiparallel configurations were used to determine the magnetoresistance, $\Delta R/R$, for the magnetic tunnel junction. The results of the magnetoresistance as a function of the applied voltage for the tunnel junction are shown in Fig. 4-15 for the experimental data as well as for the theoretical model calculations.

Fig. 4-15. Magnetoresistance as a function of the applied voltage. Black – experimental data, Red – model.

This magnetoresistance was calculated from

$$\frac{\Delta R}{R} = \frac{\tau_{parallel}}{\tau_{antiparallel}} \frac{N_{parallel}}{N_{antiparallel}} - 1$$

where the relaxation time constant was allowed to vary depending upon which magnetization orientation the magnetic tunnel junction was in.

The resistance as a function of the applied magnetic field was also measured for the tunnel junction. The experimental data was measured at 150 mV, therefore, this value for the voltage was used in the theoretical model to calculate the resistances in the parallel and antiparallel magnetization configurations. The result of the comparison of the model to the experimental data is shown in Fig. 4-16.

Fig. 4-16. Resistance area product as a function of the applied magnetic field. Black – experimental data, Red – model.

The magnetic coercivity for the transition from the parallel to the antiparallel configuration is taken to be zero and the magnetic coercivity for the transition from the antiparallel to the parallel configuration cannot be determined from the experimental data. The theoretical

model does not fit the experimental data at the field strength corresponding to the parallel and the antiparallel orientations in Fig. 4-16 because the applied voltage is very low, which is in the region where the theoretical model predicts a resistance area product which deviates from the experimental data.

Comparison with the Simmons Model

The Simmons model for the current density, J , in a tunnel junction, which neglects the effects of spin, is given in simplified form as

$$J = J_0 \left\{ \left(\varphi_0 - \frac{eV}{2} \right) \text{Exp} \left[-A \sqrt{\varphi_0 - \frac{eV}{2}} \right] - \left(\varphi_0 + \frac{eV}{2} \right) \text{Exp} \left[-A \sqrt{\varphi_0 + \frac{eV}{2}} \right] \right\}$$

where J_0 and A are defined as

$$J_0 = \frac{e}{2\pi\hbar s^2}$$

$$A = \frac{4\pi s \sqrt{2m_e}}{\hbar}$$

The resistance area product maybe found by dividing the applied voltage by the current density. The empirical parameters that fit this curve to experimental data are φ_0 and s these parameters are the insulating barrier height and thickness respectively. The same experimental data was used to fit the Simmons model. The values of the two parameters for the parallel and antiparallel configurations of the tunnel junction are shown in Table 4-4.

Table 4-4. Values for the parameters in the Simmons model used to fit to the parallel and antiparallel experimental data.

Parallel	Antiparallel
$s = 8.09 \text{ Ang}$	$s = 9.48 \text{ Ang}$
$\varphi = 2.03 \text{ eV}$	$\varphi = 1.45 \text{ eV}$

If the current density is plotted for the theoretical model, Simmons model, and the experimental data, the results give what appears to be a match for all except for the Simmons's model at higher voltages (see Fig. 4-17).

Fig. 4-17. Comparison of the new model and the Simmons model to experimental data. Black – experimental data, Red – new theoretical model, Blue – Simmons model, Triangles – antiparallel, Squares – parallel.

However, if the resistance area product is determined it is found that the curves do not generate the same shape as the experimental data. The resistance area product results of the Simmons model, the new model, and the experimental data for both the parallel and antiparallel configurations of the magnetic tunnel junction are shown in Fig. 4-18.

Fig. 4-18. Comparison of the new model and the Simmons model to experimental data. Black – experimental data, Red – new model, Blue – Simmons model, Triangles – antiparallel, Squares – parallel.

The magnetoresistance was derived for the Simmon's model by using the resistance curves for the parallel and the antiparallel configurations. The measured magnetoresistance shows a major deviation from the predictions of the Simmons model, whereas the new model proposed in this thesis gives results which are in good agreement with the experimental observations (Fig. 4-19).

Fig. 4-19. Comparison of the new model and the Simmons model to experimental data. Black – experimental data, Red – new model, Blue – Simmons model.

Discussion

The formula for the number of charge carriers needed to be changed due to the problem of electrons trying to tunnel into a section of the band in the final electrode where they were not permitted. When the formulas were first compared to the experimental data they did not have the proper shape and this problem was addressed by introducing another term. This helps to fit the model to the experimental data. The reason that this parameter was needed may be due to the oversimplification of this new model; perhaps this model is lacking a certain necessary variable. By comparing the experimental data for the resistance area product and the magnetoresistance to the results of the theoretical model it is found that they agree very well

for such a simple first approximation. However, the new model fails to describe the junction behavior at very low voltages.

Examining the experimental data and the theoretical modeling data for the resistance area product as a function of applied magnetic field it is found that the model does not follow the curve exactly. This is most likely due to the inaccurate prediction of the model for very low applied voltages. However the model equation for $R(H)$ given on pg. 43 remains valid, as shown in Fig. 4-20. This shows that if the theoretical model calculations fit the experimental data better for low voltages then the resistance area product as a function of the applied magnetic field curve would also show a better fit to the experimental data.

Fig. 4-20. Resistance area product and the applied magnetic field for the new model using the parallel and antiparallel values from the experimental data.

However, this equation does not give a “hysteresis” effect meaning if the magnetic field is changing in a positive direction the tunnel junction changes from a parallel configuration to an antiparallel configuration at a higher or lower magnetic field than if the resistance is being measured with the magnetic field changing in a negative direction. This is a recurring problem in magnetic systems, where mathematical descriptions of hysteretic effects are quite lacking. The equation does take into account the change of the antiparallel configuration to the parallel configuration at higher applied magnetic fields. This is not evident in the above data because the experimental results were not taken at high enough magnetic fields to cause this reversal. If the magnetic field were increased the model would give a result similar to Fig. 4-21.

Fig. 4-21. The magnetic field effects at high applied magnetic fields using the new model.

Comparing the results of the new magnetic tunnel junction model to the Simmons model and the experimental data for the resistance area product as a function of the applied voltage for both configurations, it appears that the new model follows the experimental results more closely; the Simmons model has too much curvature to fit properly (this can also be seen in the inset in Fig. 2-5. Another problem with the Simmons model is that it does not explain the “tail” at lower voltages; the new theoretical model does give a “tail” at these lower voltages. In this respect the model developed here represents a significant advance over previous first principles theories.

Another benefit of the new theoretical model is that if the temperature of the junction is assumed to be at absolute zero, $T = 0$ K, the equation for the resistance area product reduces to an integral that may be exactly solved analytically for the case of a finite electron band width. This is unusual because many of the integrals involved in scientific work must be solved numerically and represents an important result that can be used to help understand the behavior of magnetic tunnel junctions. The analytic solution is quite complex and it is therefore reproduced in the Appendix.

CHAPTER 5. CONCLUSIONS

Summary

A new model for magnetic tunneling junctions has been proposed and examined in this thesis. This model attempts to describe the resistance area product and magnetoresistance as a function of the applied voltage as well as the resistance area product as a function of the applied magnetic field. The model takes into account the spin polarization of the electron bands and the density of states on either side of the tunnel barrier. It has been shown how to take into account the finite width of a conduction band of the metal electrode under simplified circumstances. The model is in principle extendable to magnetic tunnel junctions with different band structures of the electrodes on either side of the junction (heterojunctions) and to include the effects of temperature.

Starting with first principles quantum mechanical considerations the equations of the model have been derived. The effects of the density of states, tunneling probability, effects of the spin polarization, magnetization configurations of the two electrodes, and the number of charge carriers has been derived and from these the equations for the current density and resistance area product were formulated.

Once the basic equations of the new theoretical model were derived they were compared with experimental data gathered from a magnetic tunnel junction supplied by Nonvolatile Electronics, Inc. The new model implements more of the underlying physics than previous models, such as the Simmons model. However taking into account the various important physical factors such as densities of states of the electrons on either side of the insulating barrier, spin polarization, and the barrier height and thickness does lead to a much more

complex model than the Simmons model. Although the basis of the model gives a more complete physical description of the processes involved in spin polarized electron tunneling, it is also apparent that the model is yet to be optimized. Initial attempts to interpret the resistance area product data were not successful for lower values of voltages. The plot of the resistance area product was corrected using a prefactor, the exact physical significance of this prefactor is yet to be determined. This prefactor reduced the resistance area product as the voltage decreased. This allowed the model equation to fit the experimental data very well (Figs. 4-12 and 4-13).

The new model was then compared to the standard model that has been used for tunnel junctions for many years – the Simmons model. Despite its simplicity, the Simmons model lacks many variables, among these it does not take into account the effects of magnetic fields or the effects of shifts in the band structure due to the exchange coupling which occur in magnetic materials. The new model presented here appears to be superior in describing the behavior of the experimental results from the magnetic tunnel junction (Figs. 4-16 and 4-17).

Benefits and Shortcomings

The new theoretical model includes important additional effects which have an important role to play in magnetic tunnel junctions. These include the effects of an applied magnetic field on magnetic tunnel junctions which the Simmons model does not contain. This is an important effect that can not be overlooked when describing the function and behavior of the magnetic tunnel junction. The new model also includes the effects of the exchange splitting in the electronic band structure caused by ferromagnetic exchange coupling which has not been included in the Simmons model. This splitting of the energies of the spin up and spin down

electron bands is derived from the exchange interaction in ordered magnetic materials such as ferromagnets that are used to form the electrodes on either side of the tunnel junction and plays a principal part in the tunneling process.

The new model emphasizes a difference between the orientations of the spins of the electrons in the electrode materials. The Simmons model assumes that the spins of the electrons do not matter, which for a magnetic tunnel junction material is clearly not the case. The magnetizations of the magnetic materials that form the electrodes is a direct result of the asymmetry in the number of spin up and spin down electrons in the conduction bands.

Although there are many positive aspects to the new magnetic tunneling model there are some aspects of the tunnel junction behavior that have not yet been explained using this model. The new theoretical model does not describe the low voltage values for both the parallel and antiparallel magnetization configurations for the measured resistances in an accurate manner. Also the negative voltage region cannot be modeled using the new theoretical model.

Future Research

The new theoretical model could be enhanced to include the effects observed for the increase of temperature. One category of this effect may be the inclusion of magnon effects. These are the effects of thermal variation on the orientations of the electron spins. For increasing temperatures the electron spins will not be fixed in a particular direction but will vary or precess around a general direction, with the degree of precession increasing with temperature. The new theoretical model should be applied to experimental results obtained on other types of tunnel junctions specifically more simple tunnel junctions where the density of states, Fermi energies, and other important properties are well known for each electrode. This could

include junctions using elemental electrodes such as a Ni/AlOx/Fe junction for example, in which the experimental results, on a junction that may not be of great practical significance, are used as a means of validation the new model.

The new model could also be tested against non-magnetic tunnel junctions such as Al/AlOx/Cu tunneling junctions. This may be done by letting the exchange energy, E_{ex} , for each electrode be exactly zero, as a special case, and comparing the experimental data to the predictions of the model equation for the resistance area product.

APPENDIX 1: PUBLISHED WORK

Simultaneous Magnetic Force Microscopy and Magnetoresistance Characterization of a Magnetic Tunnel Junction with *in-situ* Applied Field

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Abstract—For the first time, both the magneto-electronic properties and the magnetic domain structure of a magnetic tunnel junction (MTJ) have been characterized simultaneously. *In-situ* tunneling magnetoresistance measurements for a spin-dependent tunnel junction were directly compared to magnetic domain behavior imaged using magnetic force microscopy (MFM) under the same applied fields, allowing for detailed investigation of electronic behavior relative to magnetic behavior. From the results it was found that the resistance in the hysteretic field range (less than the coercivity of $H_c = 800\text{A/m}$ or 10 Oe) was correlated with the complex magnetic domain behavior observed in the MFM images.

Index Terms – Magnetic force microscopy, Domain structures, Spin dependent transport, magnetoresistance

I. INTRODUCTION

MAGNETIC tunnel junction behavior, first observed at room temperature by Moodera and co-workers [1], is currently a topic of great scientific and technological interest. The electric current through a magnetic tunnel junction relies on spin-dependent tunneling of the electrons from a ferromagnetic layer, through an insulating barrier, into another ferromagnetic layer, with the electronic spins correlated by ferromagnetic exchange forces within the magnetic domains in the ferromagnetic layers [2]. However, the true magnetic domain behavior of a spin-dependent tunnel junction as it reverses from high resistance to low resistance, and vice versa, has never been observed while the resistance is simultaneously being measured. In this paper we report results taken on a tunnel junction using a specially adapted magnetic force microscope (MFM) that can simultaneously apply magnetic fields of up to 48 KA/m (600 Oe), vary the temperature over the range -20 to $+60^\circ\text{C}$ and allow measurement of the magnetoresistance [3, 4].

The resistance of a magnetic junction depends on the relative magnetization directions in the two ferromagnetic electrodes – together with the electron band structure, and in particular the differences in the relative densities of states in the majority “spin up” half band and the minority “spin down” half band as shown in Fig.1 [5]. Parallel alignment of the magnetization in the two ferromagnetic electrodes allows the conduction electrons that tunnel through the insulating barrier layer to find conditions, such as density of states, similar on the other side. On the other hand antiparallel alignment of magnetic domains in the two electrodes means that the majority conduction electrons that tunnel through the insulating barrier, and which come from a high density of states on one side, find that the density of states is much lower on the other side. This results in a higher resistance in the antiparallel configuration.

Fig. 1 Schematic of band structures in a magnetic tunnel junction showing the majority spin up and minority spin down half bands, and how the resistance is affected by the orientation of the magnetization in the electrodes on either side of the tunneling barrier [5]

It is therefore important to determine the variation of the magnetoresistance at the same time as the magnetic domain configuration is being monitored. To this purpose a spin-dependent tunnel junction has been imaged using magnetic force microscopy while simultaneously measuring the magnetoresistance, thus allowing characterization through the entire magnetoresistance hysteresis loop.

II. Experimental Procedure

Multilayers of the structure Si(substrate)-NiFe(12nm)-AlO_x(1.5nm)-FeCo(5.4nm)-CrPrMn(32.8nm)-Al(5.4nm) were fabricated into magnetic tunnel junctions by Non-Volatile Electronics, Inc. [6]. The junctions of interest had a tapered ellipsoidal shape, with the full junction multilayer stack structure covering half the ellipsoidal area, and the other half being just the exposed NiFe free layer (divided along the long axis). Enough area of the stack and free layer were exposed from beneath Al interconnects to allow imaging by MFM. Easy axes were induced perpendicular to the ellipsoid axis by annealing under an applied magnetic field. One such multilayer device was selected and connected to a circuit via wire-bonding. The tapered half-ellipsoidal shape of this junction had dimensions of $\sim 12\mu\text{m}$ at the widest point, along the short axis and $\sim 40\mu\text{m}$ along the long axis, with the exposed bottom NiFe free layer forming the other half of the full ellipsoid. This device was then imaged on an MFM stage using a Digital Instruments Dimension 3100 AFM/MFM with CoCr-coated magnetic tips (MESP), modified to include *in-situ* applied field capability.

During imaging, a potential of 50mV was applied across the magnetic tunnel junction. For easy comparison of the junction multilayer stack to the free layer electrode, the stack was positioned in the right half of the image and the free layer in the left half. The tip of the ellipsoid from which domain nucleation began, was positioned at the top of the images. As the free layer of the junction was known to have a coercivity of $\sim 800\text{A/m}$ (10 Oe), the field was first increased to $+2.4\text{KA/m}$ (-30 Oe), decreased to -3.6KA/m (-45 Oe), and returned to $+2.4\text{KA/m}$ (+30 Oe), with domain images taken by MFM at intervals of typically 400 A/m (5 Oe),

although these intervals were deliberately chosen to be smaller when in the field range between $\pm H_C$.

III. Results and Discussion

The resistance of the junction as a function of the applied field is shown in Fig. 2. Each point on the graph corresponds to an MFM image that was taken while holding the field constant at the associated value. The hysteresis of the NiFe electrode is clearly demonstrated. The high resistance region corresponds to a magnetic field directed to the left and the low resistance region corresponds to a magnetic field directed to the right. The tunnel resistance $\Delta R/R$ was 22% for this applied voltage.

Representative images at field levels demonstrating significant changes are shown in Figs. 3 and 4, with sequentially decreasing field in Fig. 3 and sequentially increasing field in Fig. 4.

Fig. 2. Resistance of the magnetic tunnel junction as a function of applied field. H_C for the junction is ± 480 A/m (6 Oe).

Fig. 3. Magnetic force microscope images $8\ \mu\text{m}$ square of a section of tunnel junction, with NiFe free layer electrode on the left and junction multilayer stack on the right. Applied magnetic field strengths are, from left to right and top to bottom, 30, 9.9, 6.1, 3.7, 1.8, -2.8, -7.9, -14.1,

Fig. 4. Magnetic force microscope images $8\ \mu\text{m}$ square of a section of tunnel junction, with NiFe free layer electrode on the left and junction material stack on the right. Applied magnetic field strengths are, from left to right and top to bottom, -20.5, -10.5, -4.5, 1.5, 3.5, 5.5, 7.2, 11.6.

As expected, for applied fields well outside the hysteretic region, the MFM images show no magnetic contrast on either the free layer side or the multilayer stack side of the junction. For those applied fields, the magnetization of each layer is saturated in-plane, and magnetic contrast in the MFM stems from the gradient

of perpendicular component of magnetization. However, as applied field is decreased in Fig. 3 or increased in Fig. 4, domain contrast appears over both the free layer and the multilayer stack, indicating domain walls and transitions with flux coming out of the plane. Interestingly, domain contrast starts to appear before the region of steepest magnetoresistance change, at around the saturation field of the previous magnetization direction. In the region of magnetoresistance change, the domain patterns appear quite complex. These patterns are caused by the combined effects of applied magnetic field, magnetic anisotropy, and magnetostatic effects of the pointed ellipsoidal shape, the straight edge of the multilayer stack, the thin-film aspect ratio of each electrode, and the layers and their domain walls on each other. The magnetic change of the free layer is clearly not caused by simple rotation or flipping. In fact, each reversal sequence shows a domain structure that might be a vortex (see circled regions).

Also apparent is a dark band near the center of the micrographs taken at high or low fields, in both of the reversal sequences. This indicates a large field gradient, and is probably due to flux emerging from the edge of the CoFe pinned layer in the multilayer stack. At fields in the region of magnetoresistance change, where significant domain structure is observed, this band appears much lighter. In this region, there would then be ways for some of the flux to form closed paths within and between the layers, due to the domains and domain walls, with less flux emerging directly near the edge.

IV. Conclusions

This paper presents the first results of simultaneous measurement of tunneling magnetoresistance with magnetic domain imaging using magnetic force microscopy that have been reported. The study was performed on a specially adapted magnetic force microscope based on a Digital Instruments Dimension 3100 system with in-situ field capability, resistance measurement capability, and temperature control. Through simultaneous measurement of tunneling magnetoresistance, magnetic field, and domain structure, the resistance of the magnetic tunnel junction was shown to be correlated with the magnetic domain behavior of the NiFe and CoFe magnetic layers. Complex magnetic domain structures were observed over both layers in the "hysteretic" region, the region of greatest magnetoresistance change. These domain structures form as a result of the combined effects of applied field, magnetic anisotropy, and complex magnetostatic interactions. Magnetic contrast is also observed which appears to indicate flux emerging from the side of the CoFe pinned layer of the multilayer junction stack. These results indicate that while the idea of the magnetic layers in the tunnel junction being in saturated parallel or antiparallel states is a useful simple model for the devices, the actual magnetic behavior is much more complex. This is especially true in the region of changing magnetoresistance, a region of great interest for both basic understanding and technological application.

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APPENDIX 2. MATHEMATICAL RESULTS OF THE THERORETICAL MODEL

The basic objective of this section is to show that the equations for the number of charge carriers for the new theoretical model for the finite width band structure at absolute zero temperature do indeed yield an analytic solution. The solution is quite complex and therefore only the definite equations for the number of charge carriers will be given. The other equations used in the theory such as the current density, resistance area product and the magnetoresistance will be listed here as functions of the number of charge carriers for the parallel and antiparallel magnetization configurations. The definite integrals for the number of charge carriers of the two configurations are shown below.

Note: The following equations were solved using Mathematical 4.0. Therefore the notation of the variables is as follows:

D_{one} = Maximum density of states in electrode 1

E_{one} = Energy at the maximum density of states in electrode 1

E_{two} = Maximum energy of available states in electrode 1

E_{xone} = Exchange coupling energy in electrode 1

D_{two} = Maximum density of states in electrode 2

E_{onetwo} = Energy at the maximum density of states in electrode 2

E_{twotwo} = Maximum energy of available states in electrode 2

E_{xtwo} = Exchange coupling energy in electrode 2

E_F = Fermi energy

A = Parameter that includes the barrier thickness given in Chapter 3

ϕ = The average barrier height

E_x = Variable energy

eV = energy due to the applied voltage

Number of charge carriers for the parallel configuration, N_{parallel} :

$$\frac{D_{\text{one}}}{(E_{\text{one}} - E_{\text{xone}})^2 - (E_{\text{one}} - E_{\text{xone}}) * (E_{\text{two}} - E_{\text{xone}})} \int_{E_F - eV}^{E_F} \left\{ \left[(E_x + E_{\text{xone}})^2 - (E_{\text{two}} - E_{\text{xone}}) * (E_x + E_{\text{xone}}) \right] \right. \\ \left. * \text{Exp} \left[-A * \sqrt{E_F + \phi - E_x} \right] \right\} dE_x +$$

$$\frac{D_{\text{one}}}{(E_{\text{one}} + E_{\text{xone}})^2 - (E_{\text{one}} + E_{\text{xone}}) * (E_{\text{two}} + E_{\text{xone}})} \int_{E_F - eV}^{E_F} \left\{ \left[(E_x - E_{\text{xone}})^2 - (E_{\text{two}} + E_{\text{xone}}) * (E_x - E_{\text{xone}}) \right] \right. \\ \left. * \text{Exp} \left[-A * \sqrt{E_F + \phi - E_x} \right] \right\} dE_x$$

Number of charge carriers for the antiparallel configuration, $N_{\text{antiparallel}}$:

$$\frac{D_{\text{two}}}{(E_{\text{one} \text{two}} + E_{\text{xtwo}} - eV)^2 - (E_{\text{one} \text{two}} + E_{\text{xtwo}} - eV) * (E_{\text{two} \text{two}} + E_{\text{xtwo}} - eV)} \int_{E_F - eV}^{E_F} \left\{ \left[(E_x - E_{\text{xtwo}} + eV)^2 - \right. \right. \\ \left. \left. (E_{\text{two} \text{two}} + E_{\text{xtwo}} - eV) * (E_x - E_{\text{xtwo}} + eV) \right] \right. \\ \left. * \text{Exp} \left[-A * \sqrt{E_F + \phi - E_x} \right] \right\} dE_x +$$

$$\frac{D_{\text{one}}}{(E_{\text{one}} + E_{\text{xone}})^2 - (E_{\text{one}} + E_{\text{xone}}) * (E_{\text{two}} + E_{\text{xone}})} \int_{E_F - eV}^{E_F} \left\{ \left[(E_x - E_{\text{xone}})^2 - (E_{\text{two}} + E_{\text{xone}}) * (E_x - E_{\text{xone}}) \right] \right. \\ \left. * \text{Exp} \left[-A * \sqrt{E_F + \phi - E_x} \right] \right\} dE_x$$

Solving these two equations gives:

$$N_{\text{parallel}} =$$

$$\begin{aligned}
 & - \left(4 D_{\text{one}} e^{-A(\sqrt{\text{phi}} + \sqrt{\text{ev} + \text{phi}})} \right. \\
 & \quad \left(e^{A\sqrt{\text{ev} + \text{phi}}} \right. \\
 & \quad \left(A^2 \text{Exone}^2 (18 + 18 A \sqrt{\text{phi}} + A^3 (-3 \text{Ef} + \text{Etwo}) \sqrt{\text{phi}} + A^2 (-3 \text{Ef} + \text{Etwo} + 2 \text{Exone} + 6 \text{phi})) - \right. \\
 & \quad \text{Eone} (120 + 120 A \sqrt{\text{phi}} + A^5 (\text{Ef}^2 - \text{Ef} \text{Etwo} + 2 \text{Exone}^2) \sqrt{\text{phi}} + \\
 & \quad 2 A^3 \sqrt{\text{phi}} (-6 \text{Ef} + 3 \text{Etwo} + 4 \text{phi}) + 6 A^2 (-2 \text{Ef} + \text{Etwo} + 8 \text{phi}) + \\
 & \quad \left. A^4 (\text{Ef}^2 + 2 \text{Etwo} \text{phi} - \text{Ef} (\text{Etwo} + 4 \text{phi}))) \right) + \\
 & \quad e^{A\sqrt{\text{phi}}} \\
 & \quad \left(-A^2 \text{Exone}^2 (18 + 18 A \sqrt{\text{ev} + \text{phi}} + A^3 (-3 \text{Ef} + \text{Etwo} + 3 \text{ev}) \sqrt{\text{ev} + \text{phi}} + \right. \\
 & \quad \left. A^2 (-3 \text{Ef} + \text{Etwo} + 9 \text{ev} + 6 \text{phi})) + \right. \\
 & \quad \text{Eone} (120 + 120 A \sqrt{\text{ev} + \text{phi}} + A^5 (\text{Ef}^2 + \text{Etwo} \text{ev} + \text{ev}^2 - \text{Ef} (\text{Etwo} + 2 \text{ev}) + 2 \text{Exone}^2) \\
 & \quad \sqrt{\text{ev} + \text{phi}} + 2 A^3 \sqrt{\text{ev} + \text{phi}} (-6 \text{Ef} + 3 \text{Etwo} + 10 \text{ev} + 4 \text{phi}) + \\
 & \quad 6 A^2 (-2 \text{Ef} + \text{Etwo} + 10 \text{ev} + 8 \text{phi}) + \\
 & \quad \left. A^4 (\text{Ef}^2 + 3 \text{Etwo} \text{ev} + 5 \text{ev}^2 + 2 \text{Exone}^2 + 2 \text{Etwo} \text{phi} + 4 \text{ev} \text{phi} - \text{Ef} \right. \\
 & \quad \left. (\text{Etwo} + 6 \text{ev} + 4 \text{phi}))) \right) \Bigg) / (A^6 (\text{Eone} - \text{Etwo}) (\text{Eone} - \text{Exone}) (\text{Eone} + \text{Exone}))
 \end{aligned}$$

$N_{\text{antiparallel}} =$

$$\frac{1}{A^6}$$

$$\left(2e^{-A(\sqrt{\text{phi}} + \sqrt{\text{ev} + \text{phi}})} \right.$$

$\left. - \left(\text{Done} \right. \right.$

$$\begin{aligned} & \left(-e^{A\sqrt{\text{ev} + \text{phi}}} \left(120 + 120A\sqrt{\text{phi}} + A^5(Ef - \text{Etwo} - 2\text{Exone})(Ef - \text{Exone})\sqrt{\text{phi}} + \right. \right. \\ & \quad 2A^3\sqrt{\text{phi}}(-6Ef + 3\text{Etwo} + 9\text{Exone} + 4\text{phi}) + \\ & \quad 6A^2(-2Ef + \text{Etwo} + 3\text{Exone} + 8\text{phi}) + \\ & \quad A^4(Ef^2 + \text{Etwo}(\text{Exone} + 2\text{phi}) + 2\text{Exone}(\text{Exone} + 3\text{phi}) - \\ & \quad \quad Ef(\text{Etwo} + 3\text{Exone} + 4\text{phi})) \left. \right) + \\ & \quad e^{A\sqrt{\text{phi}}} \left(120 + 120A\sqrt{\text{ev} + \text{phi}} + A^5(-Ef + \text{ev} + \text{Exone}) \right. \\ & \quad \quad (-Ef + \text{Etwo} + \text{ev} + 2\text{Exone})\sqrt{\text{ev} + \text{phi}} + \\ & \quad \quad 2A^3\sqrt{\text{ev} + \text{phi}}(-6Ef + 3\text{Etwo} + 10\text{ev} + 9\text{Exone} + 4\text{phi}) + \\ & \quad \quad 6A^2(-2Ef + \text{Etwo} + 10\text{ev} + 3\text{Exone} + 8\text{phi}) + \\ & \quad \quad A^4(Ef^2 + 5\text{ev}^2 + 9\text{ev}\text{Exone} + 2\text{Exone}^2 + 4\text{ev}\text{phi} + 6\text{Exone}\text{phi} + \\ & \quad \quad \quad \text{Etwo}(3\text{ev} + \text{Exone} + 2\text{phi}) - Ef(\text{Etwo} + 6\text{ev} + 3\text{Exone} + 4\text{phi})) \left. \right) \left. \right) / \end{aligned}$$

$((\text{Eone} - \text{Etwo})(\text{Eone} + \text{Exone})) -$

$(\text{Dtwo}$

$$\begin{aligned} & \left(-e^{A\sqrt{\text{ev} + \text{phi}}} \left(120 - 6A^2(2Ef - \text{Etwo}^2 + 3\text{ev} - 3\text{Extwo} - 8\text{phi}) + 120A\sqrt{\text{phi}} + \right. \right. \\ & \quad A^5(Ef - \text{Etwo}^2 + 2\text{ev} - 2\text{Extwo})(Ef + \text{ev} - \text{Extwo})\sqrt{\text{phi}} + \\ & \quad 2A^3\sqrt{\text{phi}}(-6Ef + 3\text{Etwo}^2 - 9\text{ev} + 9\text{Extwo} + 4\text{phi}) + \\ & \quad A^4(Ef^2 + 2(\text{ev} - \text{Extwo})(\text{ev} - \text{Extwo} - 3\text{phi}) + \text{Etwo}^2(-\text{ev} + \text{Extwo} + 2\text{phi}) - \\ & \quad \quad Ef(\text{Etwo}^2 - 3\text{ev} + 3\text{Extwo} + 4\text{phi})) \left. \right) + \\ & \quad e^{A\sqrt{\text{phi}}} \left(120 + 120A\sqrt{\text{ev} + \text{phi}} + A^5(Ef - \text{Etwo}^2 + \text{ev} - 2\text{Extwo}) \right. \\ & \quad \quad (Ef - \text{Extwo})\sqrt{\text{ev} + \text{phi}} + \\ & \quad \quad 2A^3\sqrt{\text{ev} + \text{phi}}(-6Ef + 3\text{Etwo}^2 + \text{ev} + 9\text{Extwo} + 4\text{phi}) + \\ & \quad \quad 6A^2(-2Ef + \text{Etwo}^2 + 7\text{ev} + 3\text{Extwo} + 8\text{phi}) + \\ & \quad \quad A^4(Ef^2 - 2\text{ev}^2 + 5\text{ev}\text{Extwo} + 2\text{Extwo}^2 - 2\text{ev}\text{phi} + 6\text{Extwo}\text{phi} + \\ & \quad \quad \quad \text{Etwo}^2(2\text{ev} + \text{Extwo} + 2\text{phi}) - Ef(\text{Etwo}^2 + 3\text{ev} + 3\text{Extwo} + 4\text{phi})) \left. \right) \left. \right) / \end{aligned}$$

$((\text{Eonetwo} - \text{Etwo}^2)(\text{Eonetwo} - \text{ev} + \text{Extwo})) \left. \right) \left. \right)$

The current density for each of the two configurations is given as:

$$J_{parallel} = \frac{e^2 \tau V}{m_e x} N_{parallel}$$

$$J_{antiparallel} = \frac{e^2 \tau V}{m_e x} N_{antiparallel}$$

The resistance area products are given by:

$$R * A_{parallel} = \frac{m_e x}{e^2 \tau} \frac{1}{N_{parallel}}$$

$$R * A_{antiparallel} = \frac{m_e x}{e^2 \tau} \frac{1}{N_{antiparallel}}$$

The magnetoresistance is given by:

$$\frac{\Delta R}{R} = \frac{\tau_{parallel}}{\tau_{antiparallel}} \frac{N_{parallel}}{N_{antiparallel}} - 1$$

The resistance area product as a function of the applied magnetic field is given by:

$$(R * A)(H) = \left(\frac{m_e x}{2e^2 \tau} \left(\frac{1}{N_{parallel}} - \frac{1}{N_{antiparallel}} \right) \tanh \left(\frac{\mu_0 m_1 (H - H_{c1})}{kT} \right) \right) \tanh \left(\frac{\mu_0 m_2 (H - H_{c2})}{kT} \right)$$

$$+ \frac{m_e x}{2e^2 \tau} \left(\frac{1}{N_{parallel}} + \frac{1}{N_{antiparallel}} \right)$$

In the above equation m is the mass of the electron, m_1 is the magnetic moment in electrode 1, and m_2 is the magnetic moment in electrode 2.

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