The Theory of Magnetic Tunnel Junctions

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Submitted by Matthew Edward Eames, to the University of Exeter as a thesis for the degree of Doctor of Philosophy in Physics, September 2006.

I certify that all material in this thesis which is not my own work has been identified and that no material has previously been submitted and approved for the award of a degree by this or any other University.

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Abstract

Within this work an investigation into the tunnelling magnetoresistance (TMR) will be presented. A base numerical model is developed to describe the tunnelling through a magnetic tunnel junction (MTJ) so that a simple analytic model can be compared. These models have been extended to the crystalline barrier MTJs. This numerical model was based upon an enhanced Wentzel-Kramers-Brillouin (EWKB) method to describe the tunnelling current density. By correctly considering realistic MTJ parameters, the key result was found to be the correct handling of the effective masses in of the three MTJ layers. The extracted barrier-heights of 3.5-4eV is much higher than found previously and closer to the half band-gap result expected. It is then clear that the correct treatment of the parameters produces a far more realistic result. The key parameter which can be extracted from the I-V characteristics is the product $m^* d\sqrt{V_b}$, where m^* is the effective mass of the barrier, d is the effective barrier thickness and V_b is the effective barrier height.

The analytic solution is a transparent model in which the key material parameters are visible and simple enough to be applied by experimental researchers to MTJs. The accurate modelling of both the prefactor and exponent are crucial to estimating the TMR. A simplified analytic result was produced that is in good agreement with numerical and experimental results.

The numerical and analytic model are then extended to describe the TMR through a crystalline Fe(001)/MgO(001)/Fe(001) trilayer system. The calculation is based on the free-electron-like numerical solution providing a functional dependence of the TMR. The results were found to be in excellent agreement with the *ab initio* models and experiment. Furthermore a simplified analytic expression shows the TMR is dependent on the band-widths of the tunnelling electron states, the coupling and the thickness of the barrier. These models will be of great benefit to both experimental and theoretical researchers.

Acknowledgements

I would like to take this opportunity to thank the people who have helped me over the last few years towards the completion of this thesis, of which there are several.

First of all I would like to thank my supervisor John Inkson. Without his help, patience and encouragement this thesis would not exist.

There are also those who have helped me in so many other capacities both inside and outside of the office whether it's something as simple as making me tea or playing a game of tennis or squash. So I would like to thank Dan Edmunds, Paul Keatley, Nathan Maine, Steve Hepplestone, Luke Hounsome, Cathrine Blake, Jon Wills, Cathryn Hydes, Kevin Thorne, Lizzy Darnill, Suzie Burrow and Simon Masterman.

I would also like to thank my family who have always been there for me.

Finally I would like to give a special mention to Abby for all your love, support and for simply just being there for me throughout my PhD.

Thank you,
Matt

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List of Symbols

Although this list of symbols is not exhaustive, it acts as a quick reference to some of the more commonly used symbols within this thesis

B	Magnetic field
$\lvert C\rangle$	Conduction band state
d	Barrier-thickness
$D(E)$	Density of states
E_F	The Fermi energy
E_g	The energy gap between the conduction and valance bands
$E_{n,k}$	Energy of electron n with wave vector k
g	Spectroscopic splitting factor
$\hbar$	Planck's constant
H	Applied magnetic field
J	Current density
k_0	Effective wave vector of the barrier height
$\mathbf{K}$	Electron wave vector
K_B	Boltzmann's constant
l	Angular quantum number
N	Total number of electrons in a system
N_W	Molecular field
m^*	Effective mass
m_e	Free electron mass
m_l	The magnetic quantum number
m_s	The spin quantum number
n	The principle quantum number

$\hat{p}$	The momentum operator
p_i	The momentum in direction i
P	Polarisation of an electrode
q	Effective wave vector in the emitter electrode
R	Resistance
S	Conduction band / valence band mixing parameter
T	Transmission coefficient
T_C	Currie temperature
$u_{\mathbf{k}}(\mathbf{r})$	Cell periodic part of the electron wave function
U	Barrier height
V	Applied voltage
V_F	Fermi volume of the system
$V(x)$	Potential at position x
V_B	Barrier-height above the Fermi energy
$\lvert X\rangle, \lvert Y\rangle, \lvert Z\rangle$	Valence band states
α, β	Correction parameters for the Airy function transmission
$\gamma(E,V,x)$	Effective wave vector of an electron inside an insulator at energy E, voltage V and position x.
$\Gamma(E,V,d)$	Effective wave vector incorporating correction parameter α
$\mathrm{K}(E,V,x)$	Effective wave vector incorporating correction parameter β
κ	Effective wave vector of an electron inside an insulator
λ	Electron wave length
μ_B	Bohr magneton
$\phi(r)$	Potential as a function of r
χ_{spin}	Spin wave function
$\psi^n(\mathbf{r}_1)$	Wave function of electron n at position $\mathbf{r}_1$
$\psi^{n,m}(\mathbf{r}_1,\mathbf{r}_2)$	Two electron wave function at position $\mathbf{r}_1$ and $\mathbf{r}_2$

Publications

Interface scattering and the tunneling magnetoresistance of Fe(001)/Mg(O01)/Fe(001) junctions
M. E. Eames and J. C. Inkson
APPLIED PHYSICS LETTERS **88**, 252511 (2006)