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An analytic approach to tunnelling magnetoresistance

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ABSTRACT

We present an analytic model for the barrier transmission coefficient that can be used to calculate the tunnelling magnetoresistance (TMR) for metal–insulator–metal systems. It removes the approximations inherent in the Simmons' and Brinkman models currently used to fit experimental systems that give much lower predictions of the barrier height than would be expected. The model is accurate enough to directly relate to the experiment and hence device optimisation by predicting junction parameters that are in line with bulk properties.

The tunnelling magnetoresistance (TMR) effect in magnetic tunnel junctions (MTJs) describes the change of the resistance of two ferromagnetic electrodes separated by a thin insulating non-magnetic layer as the electrodes switch polarisations from parallel to antiparallel. The commonly used measure, the pessimistic TMR, is defined as $(J_p - J_{ap})/J_p$, where J_p and J_{ap} are the current density in parallel and antiparallel magnetic alignment, respectively. Each of these, in turn, are the sum of the currents resulting from tunnelling across the barrier of the majority and minority spin electrons from the anode in a given configuration. The problem for theoretical analysis is that, since the TMR depends upon calculating the difference in tunnelling currents $(J_p - J_{ap})$, a high accuracy in the calculation of each component is essential.

Approaches in use are predominantly computational; nearly free-electron-based models deriving from the work of Simmons [1] and Brinkman [2] replace the spin split bands in the contacts by free electron bands of mass m_e and the barrier by a potential barrier of a given thickness and width. This process gives a number of parameters for the system that can be suitably adjusted to fit the experimental results. The Simmons [1] and Brinkman [2] models are still used today for the determination of the barrier thickness and height of MTJ devices and analysis of TMR [3–6], even though the parameters used (effective mass, barrier heights) are often far from those expected from bulk values.

Fits to junctions with an Al_2O_3 barrier using the Simmons model have predicted barrier heights of the order 1.56 eV [7] and 2 eV [5] while the band gap of Al_2O_3 has been found to be of the order 6–10 eV [8]. Therefore, we would expect to find an extracted barrier height of at least 3–5 eV. Within each model, the effective mass within the barrier is always assumed to be the same as the effective mass within each of the electrodes. The effective mass in the barrier can vary from the free electron mass by as much as one tenth for the case of Ge [9] and even by 40% for the case of Al_2O_3 [8] increasing the probability of tunnelling through the barrier significantly compared to the tunnelling of a free electron mass.

In contrast, ab-initio calculations of MTJs are heavily computational and whilst they have proved extremely useful in dealing with crystalline barriers [10], they lack the flexibility needed to be applied to experimental systems.

Although computational approaches are extremely useful, an analytic model of the system is essential in order to explore the wide parameter range available, relate the experimental results to device parameters and optimise the TMR. This letter presents an analytic model that is accurate enough for the calculation of experimental voltage-dependent TMR ratios using realistic values for the device parameters in agreement with known band-structure values. Key to the model is an accurate formulation of the tunnelling probability through a barrier. The model presented allows for variation in material parameters in both the electrodes and the barrier while a simple extension to the Wentzel–Kramers–Brillouin (WKB) wave functions in the barrier increase the range of voltages which could be considered.

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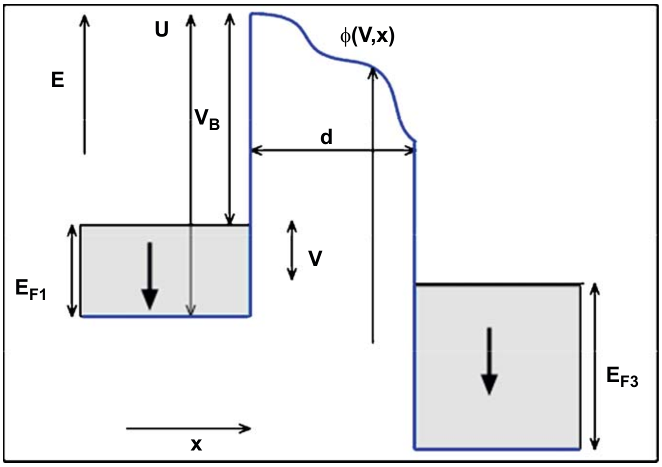

Fig. 1. Schematic of the magnetic tunnel junction showing the relevant potential parameters with applied bias V and barrier thickness d. Case shown here is for minority carrier tunnelling in an antiparallel magnetisation configuration (↓↑), where $E_{F1} < E_{F3}$.

The elements of the model are shown in Fig. 1; it builds upon the Simmons/Brinkman approach to include a more realistic parameterisation of the system. The majority and minority spin bands of the contacts are described by free electron bands with effective mass and bandwidths appropriate to the band structure of the metal involved, the insulator by a potential barrier of appropriate height, width and tunnelling effective mass. The tunnelling is assumed to maintain the carrier spin and so, depending upon whether it is parallel or antiparallel configuration, the carriers will tunnel between majority and minority bands or from majority to minority and vice versa with the appropriate transmission coefficient. The tunnelling states in the barrier are described by WKB functions. Normally this would restrict the solution to small voltages because of the behaviour of the WKB prefactor at the collector interface. By linearising the barrier potential variation near the interface and then ensuring the Airy function solutions asymptotically matching the WKB solution within the barrier [11], the voltage range can be substantially extended [12]. This method matches the wave function in the barrier to the large argument airy function (WKB approximation). By considering the exact wave function for a linear potential across the barrier and comparing with the WKB functions it is possible to correct the transmission for large applied voltage. The currents J_p and J_{ap} are then calculated by integrating over all available momentum values.

The transmission through the barrier for each spin combination s (↑↑,↓↓,↑↓,↓↑) of the MTJ is determined by solving the Schrödinger equation in three regions and matching across the boundaries. For the normal range of experimental barrier thicknesses we obtain the prefactor-exponential functional form

$$|T_s|^2 = 16\frac{m_2^2}{m_1^2}P(E,k_\perp,k_\parallel,V,d)\exp\left(-2\int_0^d \gamma(E,k_\parallel,V,x)\,dx\right), \tag{1}$$

where

$$P(E,k_\perp,k_\parallel,V,d) = \frac{k_\perp^2\left(\gamma^2(E,k_\parallel,V,d)+0.53((2m_2/\hbar^2)(V/d))^{2/3}\right)^{1/2}\gamma(E,k_\parallel,V,0)}{((m_2^2/m_1^2)k_\perp^2+\gamma^2(E,k_\parallel,V,0))((m_2^2/m_3^2)q_\perp^2+\gamma^2(E,k_\parallel,V,d)+0.40((2m_2/\hbar^2)(V/d))^{2/3})}, \tag{2}$$

$$\gamma^2(E,k_\parallel,V,x) = k_\parallel^2+\left(\frac{2m_2}{\hbar^2}\right)(U-E-\phi(V,x)), \tag{3}$$

and

$$q_\perp^2 = \frac{m_3}{m_1}k_\perp^2+\frac{2m_3}{\hbar^2}(V+(E_{F1}-E_{F3})). \tag{4}$$

$E\ (=\hbar^2/2m(k_\parallel^2+k_\perp^2))$ is the energy of the incident electron. U, V, E_{F1}, E_{F3} and $\phi\ (V,x)$ are shown in Fig. 1. U and V are the barrier offset and applied voltage, (m_1, m_2, m_3) and E_{F1}, E_{F3} are the effective masses and bandwidths in the emitter barrier and collector, respectively, appropriate to the spin combination. $k_\parallel$ is the (conserved) wave vector parallel to the interface and k and q are the wave vectors in the emitter and collector electrode, respectively. The terms in V/d arise from the WKB correction procedure. Detailed comparisons with numerical solutions show that $|T|^2$ is accurate to within 4% for all experimental voltages and material parameters relevant to TMR [12].

The tunnelling current density J_s for each spin configuration (↑↑,↓↓,↑↓,↓↑) is found in the usual way by summing over all tunnelling states.

$$J_s = \frac{e\hbar}{m_3(2\pi)^2}\left[\int_0^{\sqrt{k_F^2-k_V^2}} dk_\parallel k_\parallel \int_{\sqrt{k_F^2-k_\parallel^2-k_V^2}}^{\sqrt{k_F^2-k_\parallel^2}} dk_\perp |T_s|^2 + \int_{\sqrt{k_F^2-k_V^2}}^{k_F} dk_\parallel k_\parallel \int_0^{\sqrt{k_F^2-k_\parallel^2}} dk_\perp |T_s|^2\right], \tag{5}$$

where we define $k_V{}^2 = 2m_1V/\hbar^2$.

Since the dominant variation in the integrand is due to the exponential factor in the transmission coefficient, slowly varying prefactor P can be extracted from the integral and evaluated at an effective $\overline{k_\perp}$, $\overline{k_\parallel}$ point to give

$$J_s = \frac{e\hbar m_2}{m_3m_1(2\pi)^2d^4}\frac{\bar{q}_\perp}{\bar{k}_\perp}P(\bar{E},\bar{k}_\perp,\bar{k}_\parallel,V,d) \times \sum_{i=1,2}(-1)^{i-1}[(4d^2\Phi_i^2+6d\Phi_i+3)\exp(-2\,d\Phi_i) + (4d^2\mathrm{X}_i^2+6\,d\mathrm{X}_i+3)\exp(-2\,d\mathrm{X}_i)], \tag{6}$$

where

$$\Phi_i = \left(\frac{m_2}{m_1}\right)^{1/2}\left(k_0^2-k_F^2+(-1)^i\frac{1}{2}k_v^2\right)^{1/2}, \tag{7a}$$

$$\mathrm{X}_i = \left(\frac{m_2}{m_1}\right)^{1/2}\left(k_0^2-\left(1-\frac{m_1}{m_2}\right)k_F^2-(-1)^i\left(\frac{1}{2}-\frac{m_1}{m_2}\right)k_v^2\right)^{1/2}, \tag{7b}$$

and $k_0^2 = 2m_1U/\hbar^2$.

The contribution to the integral as a function of $k_\parallel$ peaks due to the conflicting effects of the increasing phase space and the cutoff caused by the exponential term with $k_\parallel$. The value of $k_\parallel$ at the peak in the prefactor gives an excellent fit to the current J_s evaluated numerically [12] while for all relevant values of $k_\parallel$ the variation of the prefactor is close to linear with $k_\perp$ so that

$$\bar{k}_\perp = \frac{1}{2}((k_F^2-\bar{k}_\parallel^2+k_V^2)^{1/2}+(k_F^2-\bar{k}_\parallel^2)^{1/2}), \tag{8a}$$

and

$$\bar{k}_\parallel = \sqrt{\frac{1}{2d}}\left(\frac{m_1}{m_2}-1\right)^{-1/2}\left(\frac{m_1}{m_2}(k_0^2-k_F^2)\right)^{1/4}. \tag{8b}$$