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Magnetoresistance in the ferromagnet/insulator/ferromagnet tunnel junction*

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Recently experiments and theories show that the tunnel magnetoresistance (TMR) does not only depend on the ferromagnetic metal electrodes but also on the insulator. Considering the rough-scattering effect and spin-flip effect in the insulator, this paper investigates the TMR ratio in a ferromagnet/insulator/ferromagnet (FM/I/FM) tunnelling junction by using Slonczewsik's model. A more general expression of TMR ratio as a function of barrier height, interface roughness and spin-flip effect is obtained. In lower barrier case, it shows that the TMR ratio depends on the rough-scattering effect and spin-flip effect.

Keywords: magnetoresistance, spin-flip effect, rough-scattering
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1. Introduction

Since the discovery of giant magnetoresistance[1] in magnetic superlattices, the study of spintronics or spin electronics has attracted considerable interest because of their potential applications to magnetic sensors and memory devices. Several experiments about the large ballistic magnetoresistance (BMR)[2] and the giant magnetoresistence (GMR)[3] have been reported. Recently the diluted magnetic semiconductors (DMSs)[4] have been a hot topic in this field because the discovery of its ferromagnetism. The tunnel magnetoresistance (TMR)[5] effects in systems with spin-polarized transport are at the heart of spintronics.[6] Many theoretical models have been developed to investigate the TMR effect. A simple model proposed by Julliere[7] is widely adopted, in which he made an assumption that the tunnelling current is the sum of those for spin-up and spin-down channels and the spin-flip tunnelling is absent. The conductances of polarized electrons are proportional to the product of the density of states (DOS) near the Fermi level from both magnetic electrodes for each spin channel. The relative change of the tunnelling resistance is given by $\Delta R/R = 2P_{\rm a}P_{\rm b}/(1 + P_{\rm a}P_{\rm b})$, where $P_{\rm a}$ and $P_{\rm b}$ are the conduction electron spin polarizations of the two electrodes. Another theory of the TMR was given by Slonczewski.[8] This model analyses the transmission of charge and spin currents flowing through a one-dimensional rectangular barrier separating two free-electron-like ferromagnet (FM) metals. A δ-type potential has been suggested to be the simplest description of the insulator (I) between the two FMs.[9] Both models have been widely used to explain the experimental results, and works have been done to compare these two models.[9,10] It seems that the Julliere model overestimates the values, and the Slonczewski model explains the low values of GMR observed previously.[11]

In the absence of detailed structural models of the junctions and the materials-specific electronic structures, the model suggested by Julliere focused on the factors contributing to the spin polarization, and made impossible a detailed theoretical study. While in experiment, observation of inverse TMR has been observed,[12] which shows that the transport properties of TMR depend not only on the ferromagnetic metal electrodes but also on the insulator. And rough interface scattering and spin-flip effects[13] will change the transport current. In this paper, using the model of Slonczewski and a δ-type potential, we will investigate the TMR in a ferromagnet/insulator/ferromagnet (FM/I/FM) tun-

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nelling junction. We consider the spin-flip and scattering roughness effect in the insulator. In higher potential barrier, it can reproduce precious result obtained in Ref.[9], while in lower potential barrier the TMR ratio is affected by the interface roughness and the spin-flip effect.

2. The spin-polarized tunnelling model

Let us consider a FM/I/FM trilayer structure of two ferromagnetic layers separated by a very thin insulating layer. The layers are assumed to be $x-y$ plane and to be stacked along the z direction. Gao *et al*[11] have demonstrated that there is only small difference between the magnitude of TMR calculated by using the δ-type potential and the rectangular potential while the δ-type potential leads the calculation simplified. In this paper, we choose the thin insulating layer as a δ-type potential. Without considering the thickness of the insulator, the effect of the insulator disorder on the transverse momentum will not be considered. We will consider this effect in our further study.

When considering the rough interface, by using the Green function method, Dong *et al*[14] have demonstrated that its effect can be modelled as an imaginary non-Hermitian Hamiltonian. This non-Hermitian Hamiltonian leads the current unconserved in the z-direction, which can be attributed to the fact that the roughness scatters the z-direction current to other direction. Because when using the Green function method, we only consider small rough scattering effect, the unconserved current in z-direction is very small in comparison with the total current. Considering the spin-flip effect, we can model the potential at the insulator interface as $U(\boldsymbol{r}) = U\delta(z)$ at $z = 0$, where U is composed of three parts and it can be written as

$$U = U_1\begin{bmatrix}1&0\\0&1\end{bmatrix} + U_2\begin{bmatrix}0&1\\1&0\end{bmatrix} - \mathrm{i}U_3\begin{bmatrix}1&0\\0&1\end{bmatrix}, \tag{1}$$

where U_1 describes the normal barrier height and width, U_2 the spin-flip effect and U_3 the rough-interface scattering height effect. With the free-electron approximation of the spin-polarized conduction electrons, the effective one-electron Hamiltonian is give by

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + U\delta(z) - h(z)\cdot\sigma. \tag{2}$$

Here the first term on right-hand side is the kinetic energy, the second one is the potential energy of equation (1), and the third one is the internal exchange energy with $h(z)$ the molecular field and σ the conventional Pauli spin operator.

Consider a spin-up electron incident on the barrier from the left FM, by matching value and slope of wave functions across the barrier, one finds that this incident electron will produce four sets of quasiparticle wave: spin-up and spin-down electrons reflected in the left FM, and spin-up and spin-down electrons transmitted into the right FM. It is worth to point out here that a spin-up incident plane wave can generate a spin-down reflecting wave due to the change in spin quantization axis. This phenomenon is similar to the well-known Andreev reflection,[15] which occurs in normal-metal-insulator-superconductor junctions, although their mechanisms are different. The wave functions on both sides of the barrier are given by

$$\psi_{\mathrm{A}}(z) = \begin{bmatrix}1\\0\end{bmatrix}\mathrm{e}^{\mathrm{i}k^{\mathrm{a}}_{z\uparrow}z} + R_\uparrow\begin{bmatrix}1\\0\end{bmatrix}\mathrm{e}^{-\mathrm{i}k^{\mathrm{a}}_{z\uparrow}z} + R_\downarrow\begin{bmatrix}0\\1\end{bmatrix}\mathrm{e}^{-\mathrm{i}k^{\mathrm{a}}_{z\downarrow}z}, \tag{3}$$

$$\psi_{\mathrm{B}}(z) = C_\uparrow\begin{bmatrix}1\\0\end{bmatrix}\mathrm{e}^{\mathrm{i}k^{\mathrm{b}}_{z\uparrow}z} + C_\downarrow\begin{bmatrix}0\\1\end{bmatrix}\mathrm{e}^{\mathrm{i}k^{\mathrm{b}}_{z\downarrow}z}, \tag{4}$$

where the k^{a}_{zs} and k^{b}_{zs} with $s =\uparrow$ and $\downarrow$ are the z-direction wave vectors, with $\hbar k_\uparrow = \sqrt{2mE}$ and $\hbar k_\downarrow = \sqrt{2m(E-\Delta)}$, E is the energy of the electron and $\Delta = 2h$. R_s and C_s are coefficients to be determined by boundary conditions. Considering that the two FMs have different M directions, we use the following spin transformation matrix:

$$\hat{T} = \begin{bmatrix}\cos\dfrac{\theta}{2} & \sin\dfrac{\theta}{2}\\ -\sin\dfrac{\theta}{2} & \cos\dfrac{\theta}{2}\end{bmatrix}, \tag{5}$$

where θ is the angle between the magnetizations of the two FMs. Then boundary conditions at $z = 0$ can be written as

$$\psi_{\mathrm{A}}(0) = \hat{T}\psi_{\mathrm{B}}(0), \tag{6}$$

$$\left(\frac{\partial\psi_{\mathrm{A}}}{\partial z}\right)_{z=0} + \frac{2mU_1}{\hbar^2}\psi_{\mathrm{A}}(0) + \frac{2mU_2}{\hbar^2}\begin{bmatrix}0&1\\1&0\end{bmatrix}\psi_{\mathrm{A}}(0) - \mathrm{i}\frac{2mU_3}{\hbar^2}\begin{bmatrix}1&0\\0&1\end{bmatrix}\psi_{\mathrm{A}}(0) = \hat{T}\left(\frac{\partial\psi_{\mathrm{B}}}{\partial z}\right)_{z=0}. \tag{7}$$

After tedious calculation, we find

$$C_\uparrow(0) = 2k^{\rm a}_{z\uparrow}(k^{\rm a}_{z\downarrow} + k^{\rm b}_{z\downarrow} + Q_3 + {\rm i}Q_1]/D(0), \quad (8)$$

$$C_\uparrow(\pi) = 2{\rm i}k^{\rm a}_{z\uparrow}Q_2/D(\pi), \quad (9)$$

$$C_\downarrow(0) = 2{\rm i}k^{\rm a}_{z\uparrow}Q_2/D(0), \quad (10)$$

$$C_\downarrow(\pi) = 2k^{\rm a}_{z\uparrow}(k^{\rm a}_{z\downarrow} + k^{\rm b}_{z\uparrow} + Q_3 + {\rm i}Q_1]/D(\pi), \quad (11)$$

where

$$D(0) = (k^{\rm a}_\uparrow x + k^{\rm b}_\uparrow x + Q_3 + {\rm i}Q_1) \times (k^{\rm a}_\downarrow x + k^{\rm b}_\downarrow x + Q_3 + {\rm i}Q_1) + Q_2^2, \quad (12)$$

$$D(\pi) = (k^{\rm a}_\uparrow x + k^{\rm b}_\downarrow x + Q_3 + {\rm i}Q_1) \times (k^{\rm a}_\downarrow x + k^{\rm b}_\uparrow x + Q_3 + {\rm i}Q_1) + Q_2^2, \quad (13)$$

and $Q_i = 2mU_i/\hbar^2$, $i = 1, 2, 3$. For a spin-down incident wave from the left FM, similar expression can be obtained with

$$C'_\uparrow(0) = 2{\rm i}k^{\rm a}_{z\downarrow}Q_2/D(0), \quad (14)$$

$$C'_\uparrow(\pi) = 2k^{\rm a}_{z\downarrow}(k^{\rm a}_{z\uparrow} + k^{\rm b}_{z\downarrow} + Q_3 + {\rm i}Q_1]/D(\pi), \quad (15)$$

$$C'_\uparrow(0) = 2k^{\rm a}_{z\uparrow}(k^{\rm a}_{z\uparrow} + k^{\rm b}_{z\downarrow} + Q_3 + {\rm i}Q_1]/D(0), \quad (16)$$

$$C'_\downarrow(\pi) = 2{\rm i}k^{\rm a}_{z\downarrow}Q_2/D(\pi). \quad (17)$$

3. Results and discussions

In the absence of applied voltage all the electrons are at equilibrium state and there is no net tunnelling current. When a small voltage V is applied, a nonequilibrium electron population will be generated. For a small voltage, the charge-current density across the tunnelling barrier can be evaluated by[16]

$$J = J_\uparrow + J_\downarrow = -{\rm e}^2V\Big[\int \frac{{\rm d}^3k^{\rm b}_\uparrow}{(2\pi)^3}\frac{\partial f_0(E^{\rm b}_\uparrow)}{\partial E^{\rm b}_\uparrow}(|C_\uparrow|^2 + |C'_\uparrow|^2)v^{\rm b}_{z\uparrow} + \int \frac{{\rm d}^3k^{\rm b}_\downarrow}{(2\pi)^3}\frac{\partial f_0(E^{\rm b}_\downarrow)}{\partial E^{\rm b}_\downarrow}(|C_\downarrow|^2 + |C'_\downarrow|^2)v^{\rm b}_{z\downarrow}\Big], \quad (18)$$

where $v^{\rm b}_{zs} = \hbar k^{\rm b}_{zs}/m$, and $f_0(E^{\rm b}_s)$ is the equilibrium distribution function of conduction electrons with energy $E^{\rm b}_s$ and spin s. The triple momentum integral in Eq.(19) is readily reduced to a single one by changing the integration variables to the spheroidal coordinates, and under the approximate relation $\partial f_0/\partial E^{\rm b}_s \simeq -\delta(E^{\rm b}_s - E_{\rm F})$ for low temperatures ($k_{\rm B}T \ll E_{\rm F}$), we only need to calculate these electrons near Fermi sphere, then we will get

$$J = -\frac{e^2V}{\hbar(2\pi)^2}\Big[\int_0^{k_{\rm F\uparrow}} k{\rm d}k(|C_\uparrow|^2 + |C'_\uparrow|^2) + \int_0^{k_{F\downarrow}} k{\rm d}k(|C_\downarrow|^2 + |C'_\downarrow|^2)\Big], \quad (19)$$

where $k_{{\rm F}\delta}$ is the Fermi vector at the Fermi sphere.

The tunnelling conductance is defined by $\sigma(\theta) = J(\theta)/V$, which is θ dependent because all the coefficients are θ dependent. We can get

$$\sigma(0) = \frac{e^2}{4\pi^2\hbar} \times \{[(k^{\rm b}_\uparrow k^{\rm a}_\uparrow)^2 I(k^{\rm b}_\uparrow + k^{\rm a}_\uparrow) + (k^{\rm b}_\downarrow k^{\rm a}_\downarrow)^2 I(k^{\rm b}_\downarrow + k^{\rm a}_\downarrow)] + [(k^{\rm b}_\uparrow k^{\rm a}_\downarrow)^2 + (k^{\rm b}_\downarrow k^{\rm a}_\uparrow)^2]I'(k^{\rm b}_\downarrow + k^{\rm a}_\downarrow)]\}, \quad (20)$$

$$\sigma(\pi) = \frac{e^2}{4\pi^2\hbar} \times \{[(k^{\rm b}_\uparrow k^{\rm a}_\downarrow)^2 I(k^{\rm b}_\uparrow + k^{\rm a}_\downarrow) + (k^{\rm b}_\downarrow k^{\rm a}_\uparrow)^2 I(k^{\rm b}_\downarrow + k^{\rm a}_\uparrow)] + [(k^{\rm b}_\downarrow k^{\rm a}_\downarrow)^2 + (k^{\rm b}_\uparrow k^{\rm a}_\uparrow)^2]I'(k^{\rm b}_\downarrow + k^{\rm a}_\uparrow)\}, \quad (21)$$

where $I(k) = \int_0^1 \frac{4x^3[(Q_1^2a + bc)^2 + Q_1^2(Q_2^2 - Q_1^2 - b^2)^2]}{[Q_1^2(a^2 + b^2) - 2Q_1^2Q_2^2 + c^2]^2}{\rm d}x$
with $a = kx + Q_3$, $b = (K - k)x + Q_3$, $c = kx^2(K - k) + KxQ_3 + Q_3^2 + Q_2^2$, $K = k^{\rm a}_\uparrow + k^{\rm a}_\downarrow + k^{\rm b}_\uparrow + k^{\rm b}_\downarrow$ and $I'(k) = \int_0^1 \frac{4x^3}{Q_1^2(a^2 + b^2) - 2Q_1^2Q_2^2 + c^2}{\rm d}x$.

The maximal TMR can be defined as $\Delta R_{\max}/R = [\sigma(0) - \sigma(\pi)]/\sigma(0)$. As a result, we can get

$$\frac{\Delta R}{R} = 1 - \frac{(k^{\rm b}_\uparrow k^{\rm a}_\downarrow)^2 I(k^{\rm b}_\uparrow + k^{\rm a}_\downarrow) + [(k^{\rm b}_\downarrow k^{\rm a}_\downarrow)^2 + (k^{\rm b}_\uparrow k^{\rm a}_\uparrow)^2]I'(\pi) + (k^{\rm b}_\downarrow k^{\rm a}_\uparrow)^2 I(k^{\rm b}_\downarrow + k^{\rm a}_\uparrow)}{(k^{\rm b}_\uparrow k^{\rm a}_\uparrow)^2 I(k^{\rm b}_\uparrow + k^{\rm a}_\uparrow) + [(k^{\rm b}_\downarrow k^{\rm a}_\uparrow)^2 + (k^{\rm b}_\uparrow k^{\rm a}_\downarrow)^2]I'(0) + (k^{\rm b}_\downarrow k^{\rm a}_\downarrow)^2 I(k^{\rm b}_\downarrow + k^{\rm a}_\downarrow)}. \quad (22)$$

In the case of high barrier when $Q_1 \gg 2k^{\rm b}_\uparrow$, the approximate TMR ratio in Ref.[8] can also be obtained as

$$\frac{\Delta R}{R} = \frac{2P_{\rm a}P_{\rm b}}{1 + P_{\rm a}P_{\rm b}}, \quad (23)$$

where

$$P_{\rm a} = \frac{(k^{\rm a}_\uparrow)^2 - (k^{\rm a}_\downarrow)^2}{(k^{\rm a}_\uparrow)^2 + (k^{\rm a}_\downarrow)^2}. \quad (24)$$

The expression for $P_{\rm b}$ is identical to Eq.(15) except that subscript a is replaced by b as in Ref.[9].

We now study how the insulator barrier affects the TMR ratio. The barrier height is characterized by Q_1, the spin-flip effect by Q_2 and the interface roughness by Q_3. In numerical calculation we take $k_\downarrow^2/k_\uparrow^2 = 0.48$. First, we investigate the effects of barrier height and the spin-flip effect when there is no interface roughness ($Q_3 = 0$). Figure 1 shows the TMR ratio, together with tunnelling conduction $\sigma(0)$ and $\sigma(\pi)$, as a function of the barrier strength for three fixed values of Q_2. When the barrier height is low, the TMR ratio changes from negative to positive and the conductance $\sigma(0)$ and $\sigma(\pi)$ decrease after a maximum with the increasing of Q_1. This result can be attributed to the facts that the spin-dependent tunnelling gives rise to a difference in conductances between the parallel (P) and anti-parallel (AP) arrangements of the magnetizations to the two FMs and that the spin-conserving and spin-flip tunnelling processes have the opposite effect on TMR. For the spin-conserving tunnelling process, the P arrangement yields much higher conductance through the barrier than that of the AP arrangement,

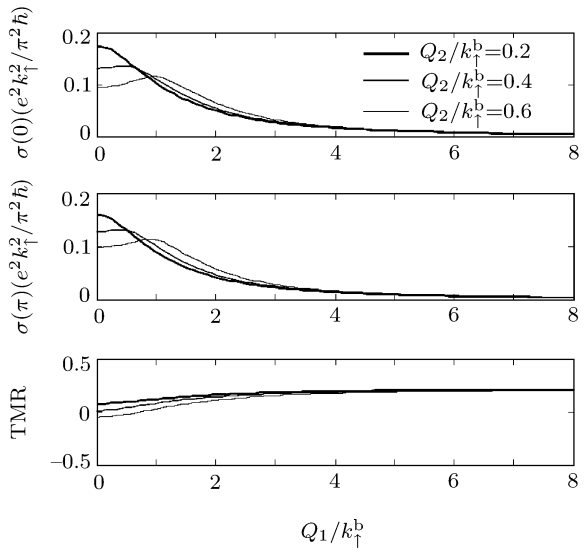


Fig.1. The TMR ratio, together with tunnelling conduction $\sigma(0)$ and $\sigma(\pi)$, as a function of the barrier strength when $Q_3 = 0$ where $k_\downarrow^2/k_\uparrow^2 = 0.48$.

leading to a large negative TMR. For the spin-flip tunnelling process, however, the situation is quite the opposite. With the increase of Q_1, the spin-conserving tunnelling becomes larger, and the TMR ratio changes from negative to positive.

Secondly, we investigate the effects of barrier height and the interface roughness when there is no spin-flip effect ($Q_2 = 0$). Figure 2 shows that with the increase of Q_1 and Q_2, the tunnelling conduction $\sigma(0)$ and $\sigma(\pi)$ decrease and the TMR ratio increases. It shows that the roughness affects the TMR ratio and adds the spin-conserving process.

While in higher barrier ($Q_1 \gg 2k_\uparrow^{\rm b}$) case, the TMR ratio magnitude is almost unchanged with Q_1, Q_2 and Q_3 as shown in Fig.1 and Fig.2. From equation (23), we can find that the electron wave vectors of the two FMs determine the TMR ratio.

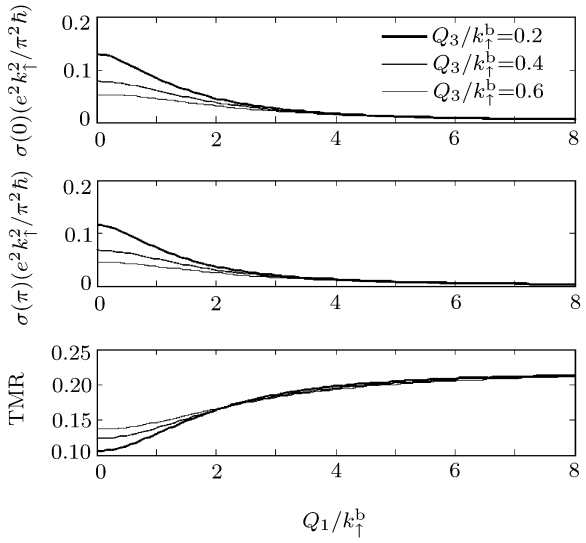


Fig.2. The TMR ratio, together with tunnelling conduction $\sigma(0)$ and $\sigma(\pi)$, as a function of the barrier strength when $Q_2 = 0$ where $k_\downarrow^2/k_\uparrow^2 = 0.48$.

In summary, we have studied the tunnelling magnetoresistance in the FM/I/FM tunnel junction when there are the rough-scattering effect and spin-flip effect. In lower barrier case, the TMR ratio changes with the rough scattering effect and the spin-flip effect, which shows that the TMR ratio depends on the insulator. While in higher barrier case, the electron wave vectors are more important in determining the TMR ratio.

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