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Structure dependence of the tunnel magnetoresistance in junctions with three ferromagnetic layers

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Abstract
We investigate theoretically the hysteresis loop and the tunnel magnetoresistance (TMR) for junctions with three ferromagnetic layers. The layers are separated by two barriers and coupled magnetically. The hysteresis curves are determined from the Heisenberg model. If the interaction between the middle layer and one of the other layers is antiferromagnetic, under a range of applied field the polarization of the middle layer can be opposite to those of the other layers. In this case the TMR ratio can be enhanced due to the difference in transmission between electrons with majority and minority spins. The results obtained are in good agreement with recent experimental results. We also discuss the possibility of optimizing the TMR ratio by tuning the thickness of the middle layer.

1. Introduction

The tunnel magnetoresistance (TMR) in planar junctions consisting of two ferromagnetic (FM) layers separated by a thin insulating barrier has been studied extensively for several years [1–3]. In the efforts to enhance the TMR ratio of the fabricated devices, the effect of a FM-doped film added within the barrier has attracted a lot of attention. Although several samples with FM dopants in the insulator exhibit reduction of the TMR ratio [4], enhancement of the TMR ratio in the Fe-doped Al_2O_3 barrier and in junctions with three FM layers was reported [5–7]. Usually the variation of the magnetization of the middle FM layer on changing the magnetic field has a crucial effect on the value of the TMR ratio. Thus, it is interesting to investigate theoretically the features of the magnetic hysteresis and their effects on the tunnelling of electrons.

In this paper we investigate the hysteresis loop and the conductance for junctions with three ferromagnetic layers. The layers are separated by two barriers and coupled magnetically. Using the Heisenberg model, the hysteresis curves are calculated. It is found that if the interaction between the middle layer and one of the other layers is antiferromagnetic, under a range of applied field the polarization of the middle layer can be opposite to those of the other layers.

In this case the TMR ratio can be enhanced due to the difference in transmission between electrons with majority and minority spins. The results obtained are in good agreement with recent experimental results. We also discuss the possibility of optimizing the TMR ratio by tuning the thickness of the middle layer.

The paper is organized as follows. In the next section we calculate the hysteresis curves of the three-layer structure. The conductance and TMR ratio are investigated in section 3. A brief summary and a discussion are presented in the last section.

2. The Heisenberg model and hysteresis curves for junctions with three FM layers

We first study the hysteresis loop for the junctions with three FM layers on varying the magnetic field. We write the Hamiltonian of the magnetic system as

$$\mathcal{H} = \sum_{j=1}^{3} \mathcal{H}_j + \mathcal{H}_C \tag{1}$$

where the $\mathcal{H}_j$ with $j = 1, 2$, and 3 are the sub-Hamiltonians of the left, middle, and right FM layers, respectively, and $\mathcal{H}_C$ is the magnetic coupling between them. In order to include the domain structure in FM layers that is crucial to the formation of the hysteresis loop and the coercive field, we use the Heisenberg model to describe the magnetic interactions among the moments of magnetic domains [8]:

$$\mathcal{H}_j = -\sum_{\boldsymbol{r},\boldsymbol{r}'\in j} J_{\boldsymbol{r}\boldsymbol{r}'} \boldsymbol{M}_{\boldsymbol{r}} \cdot \boldsymbol{M}_{\boldsymbol{r}'} - \sum_{\boldsymbol{r}\in j} \boldsymbol{B} \cdot \boldsymbol{M}_{\boldsymbol{r}} \tag{2}$$

$$\mathcal{H}_C = -\sum_{j=1,2} \sum_{\boldsymbol{r}\in j,\boldsymbol{r}'\in j+1} J_{\boldsymbol{r}\boldsymbol{r}'} \boldsymbol{M}_{\boldsymbol{r}} \cdot \boldsymbol{M}_{\boldsymbol{r}'} \tag{3}$$

where $\boldsymbol{M}_{\boldsymbol{r}}$ is the moment of domain at position $\boldsymbol{r}$, $J_{\boldsymbol{r}\boldsymbol{r}'}$ is the exchange interaction between $\boldsymbol{M}_{\boldsymbol{r}}$ and $\boldsymbol{M}_{\boldsymbol{r}'}$, and $\boldsymbol{B}$ is the field. We use the direction of the external field as the polarization axis. We assume that the statistical average of the projection of $\boldsymbol{M}_{\boldsymbol{r}}$ on this axis is constant throughout a layer:

$$\langle M_{\boldsymbol{r}} \rangle_j \equiv M_j \langle \cos\theta_{\boldsymbol{r}} \rangle_j \qquad \text{for } \boldsymbol{r} \in j \tag{4}$$

where $\theta_{\boldsymbol{r}}$ is the angle between the moment and the axis, and M_j is the average domain moment in layer j. From the mean-field treatment the average polarization can be expressed as

$$\langle \cos\theta_{\boldsymbol{r}} \rangle_j = \left(\int_{-1}^{1} \mathrm{d}x \; x \mathrm{e}^{(h_j+B)M_j x/k_B T} \right) \Big/ \left(\int_{-1}^{1} \mathrm{d}x \; \mathrm{e}^{(h_j+B)M_j x/k_B T} \right) \tag{5}$$

where $h_j = \sum_{j'} \lambda_{jj'} M_{j'} \langle \cos\theta_{\boldsymbol{r}} \rangle_{j'}$, T is the temperature, k_B is the Boltzmann constant, and

$$\lambda_{jj'} = \sum_{\boldsymbol{r}'\in j'} J_{\boldsymbol{r}\boldsymbol{r}'} \qquad \text{for } \boldsymbol{r} \in j.$$

Since the layers are ferromagnetic, $\lambda_{jj} > 0$. The signs of λ_{12} and λ_{23} depend on the nature of the barriers between the layers. They may be antiferromagnetic or weakly ferromagnetic. The value of λ_{jj} ($j = 1, 2, 3$) can be estimated from the corresponding Curie temperature:

$$\lambda_{jj} = \frac{3k_B T_{cj}}{M_j^2} \tag{6}$$

where T_{cj} is the Curie temperature of the jth layer when it is isolated from the others. The strength of the inter-layer interactions depends on the nature of the barriers and is usually smaller than that of the interactions within one layer. In the following we use $k_B T_{c1}/M_1^2$ as the unit of $\lambda_{jj'}$. The domain moments M_j are phenomenological parameters determined by the species in the layers as well as by the process of manufacture of the device. For simplicity we set $M_j \equiv M$ for $j = 1, 2, 3$, and the value of M may be obtained from the coercive field of the sample. At the same time the values of T_{c2}/T_{c1} and T_{c3}/T_{c1} are chosen in accordance with the species and thickness.

At the beginning a strong field is applied to the sample so that the polarizations of all layers are saturated and along the direction of the field. By decreasing and then reversing the field, the polarization of the layers is reversed. In this process $\langle M_r \rangle_j$ in every layer can be determined from equation (4) and the average magnetization of the whole system can be calculated as

$$\langle M_r \rangle = \left(\sum_j l_j \langle M_r \rangle_j \right) \Big/ L \tag{7}$$

where l_j is the thickness of the jth layer and $L = \sum_j l_j$. In the inverse process of varying the field, another branch of the hysteresis is obtained. The calculated hysteresis loop is illustrated in figure 1. It can be seen that the polarization is reversed at different coercive fields for different layers. The plateaus represent stable configurations of polarizations. This figure is in good agreement with figure 1 of reference [6]. The domain moment M can be determined from the coercive field shown in reference [6] as $M \sim 1.8 \times 10^2\ \mu_B$ with μ_B the Bohr magneton.

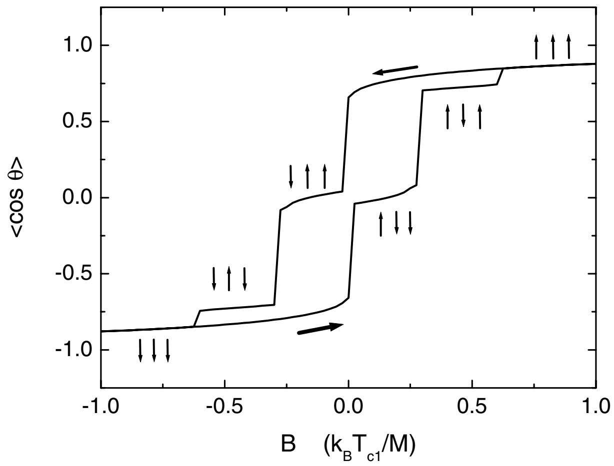

Figure 1. The hysteresis loop for junctions with three layers on varying the applied field. The FM exchange interactions within layers 1 and 3 are the same ($T_{c3} = T_{c1}$). The temperature is $T = 0.37T_{c1}$. The other exchange interactions are $\lambda_{22} = 3.67k_BT_{c1}/M^2$, $\lambda_{12} = -0.67k_BT_{c1}/M^2$, and $\lambda_{23} = 0.083k_BT_{c1}/M^2$. The thicknesses of the layers are as follows: $l_1/L = l_3/L = 0.46$; $l_2/L = 0.08$.

We note that in figure 1 the coupling between the left and the middle layers is anti-ferromagnetic-like while that between the middle and the right layers is ferromagnetic-like. This leads to the possibility of the first conversion of polarization of the left layer in reversing the field. At the same time the FM exchange interaction within the middle layer is strong, ensuring that the polarization of this layer is the last one to be converted. As a result, under a range of the applied field the polarization of the middle layer is kept unchanged while the polarizations of the left and right layers are both converted, as observed in the experiments of references [6] and [7]. The strong FM exchange interaction of the middle layer can be obtained if the crystalline structure of this layer is not substantially destroyed by atomic diffusion or lattice mismatching. In contrast, if the middle layer does not have a complete structure, or is just some atomic planes in the insulator doped with FM ions, the FM exchange interaction within it is weak and it should be the first one to be converted on changing the field. This situation is shown in figure 2. The coercive field for the middle layer is even negative if the exchange interactions between this layer and the outside layers are both antiferromagnetic. In this case the configuration with the polarization of the middle layer opposite to those of the outside layers (↓↑↓) also exists for a range of field. It can be seen that this range is reduced if the exchange interaction between layers 2 and 3 is changed from antiferromagnetic to ferromagnetic.

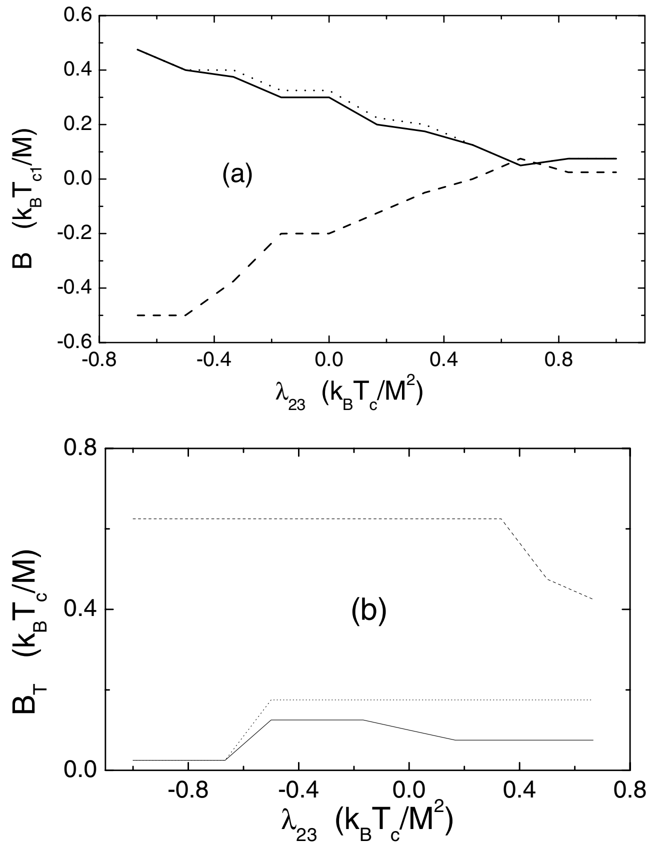

Figure 2. The coercive fields as functions of λ_{23} for the left (solid lines), middle (dashed lines), and right (dotted lines) layers. (a) $\lambda_{22} = 1.67k_BT_{c1}/M^2$, (b) $\lambda_{22} = 3.67k_BT_{c1}/M^2$. The other parameters are the same as for figure 1.

3. Conductance and TMR ratio

Now we investigate the TMR ratio in such three-layer structures. The main difference from the ordinary two-layer structures is the existence of the middle layer with polarization opposite to those of the other layers. In a free-electron approximation the longitudinal part of the effective one-electron Hamiltonian can be written [9] as

$$\mathcal{H}_z = -\frac{1}{2}(\mathrm{d}/\mathrm{d}z)^2 + U(z) - b(z)\sigma \tag{8}$$

where the system of units incorporates unit electron mass and unit Planck constant, $\sigma = \pm$ is the spin of the electron, $h(z) = B_j^E$ for z within the jth layer and zero in the barriers with $B_j^E = \lambda M \langle \cos\theta_r \rangle_j$ which is the effective magnetic field felt by the electron, $U(z) = U_0$ for z within the barriers, and $U(z) = U_2$ for z in the middle FM layer corresponding to the difference of the band bottom of this layer from those of the left and right layers. U_2 depends on the species and environment of the middle layer. The potential profile is plotted in figure 3 for spin-up and spin-down electrons in the configuration $\uparrow\downarrow\uparrow$. Although the transverse momentum $\boldsymbol{k}_\parallel$ does not appear, the final results are summations over $\boldsymbol{k}_\parallel$.

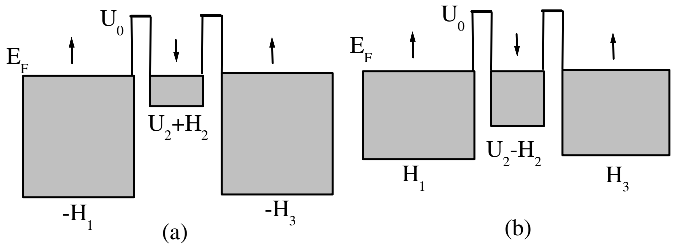

Figure 3. The potential profile for spin-up (a) and spin-down (b) electrons in an $\uparrow\downarrow\uparrow$ configuration.

We note that the left and right layers are much thicker than the middle one. Consider a wave of electrons having spin σ and unit incident particle flux injected into the left layer. The longitudinal wave function can be written as

$$\psi_\sigma(z) = \begin{cases} k_{1\sigma}^{-1/2} \exp(\mathrm{i}k_{1\sigma} z) + r_\sigma \exp(-\mathrm{i}k_{1\sigma} z) & z \leqslant b_1 \\ A_{j\sigma} \exp(\kappa z) + B_{j\sigma} \exp(-\kappa z) & b_j < z < a_{j+1} \\ C_\sigma \exp(\mathrm{i}k_{2\sigma} z) + D_\sigma \exp(-\mathrm{i}k_{2\sigma} z) & a_2 < z < b_2 \\ t \exp(\mathrm{i}k_{3\sigma} z) & z \geqslant a_3 \end{cases} \tag{9}$$

where

$$k_{2\sigma} = \sqrt{2(E_z - U_2 + B_2^E \sigma)}$$
$$k_{j\sigma} = \sqrt{2(E_z + B_j^E \sigma)} \qquad \text{for } j = 1, 3$$
$$\kappa = \sqrt{2(U_0 - E_z)}$$

with E_z the energy of the electron subtracted from the transverse kinetic energy. The coefficients can be solved from the continuity conditions at interfaces for the wave function and its first derivative. The particle transmissivity is then calculated as [9]

$$T_p = \mathrm{Im} \sum_\sigma \psi_\sigma^* \frac{\mathrm{d}\psi_\sigma}{\mathrm{d}z}. \tag{10}$$

We obtain the conductance by summing over the transverse momentum and the longitudinal energy:

$$G \propto - \sum_{k_\parallel} \sum_{E_z} T_p \frac{\partial f(E)}{\partial E} \tag{11}$$

where $f(E) = 1/\{1 + \exp[(E - E_F)/k_B T]\}$ with $E = E_z + k_\parallel^2/2$ and E_F the Fermi energy.

If the damping of the wave function in the barriers is strong enough that $\exp(-\kappa\delta_1) \ll 1$ and $\exp(-\kappa\delta_2) \ll 1$ with δ_1 and δ_2 the thicknesses of the first and second barriers, respectively, the transmissivity can be approximately expressed as

$$T_p = \sum_{\sigma} \frac{1}{(\kappa^2 + k_{1\sigma}^2)(\kappa^2 + k_{3\sigma}^2)} \frac{64\kappa^4 k_{1\sigma} k_{2\sigma}^2 k_{3\sigma} \mathrm{e}^{-2\kappa(\delta_1+\delta_2)}}{[(\kappa^2 - k_{2\sigma}^2)\sin(k_{2\sigma}d) + 2k_{2\sigma}\kappa\cos(k_{2\sigma}d)]^2} \tag{12}$$

where d is the thickness of the middle FM layer.

As shown in the last section, in structures with three FM layers there are several different configurations of layer polarizations on varying the field. The resistance depends on the configuration, leading to the TMR ratio. We calculate the TMR ratio as

$$R(B) = \frac{G^{-1}(B) - G^{-1}(B \to \infty)}{G^{-1}(B \to \infty)} \tag{13}$$

where $G(B)$ is obtained from equation (11) in the spin configuration under external field B. In figure 4 we show the calculated TMR ratio as a function of the applied field in a hysteresis loop. The effective field felt by electron spins in every layer is obtained from the polarization calculated in the last section. The curve is in good agreement with figure 3 of reference [6]. Two plateaus of TMR values correspond to two spin configurations: $\downarrow\uparrow\uparrow$ (or $\uparrow\downarrow\downarrow$) and $\downarrow\uparrow\downarrow$ (or $\uparrow\downarrow\uparrow$).

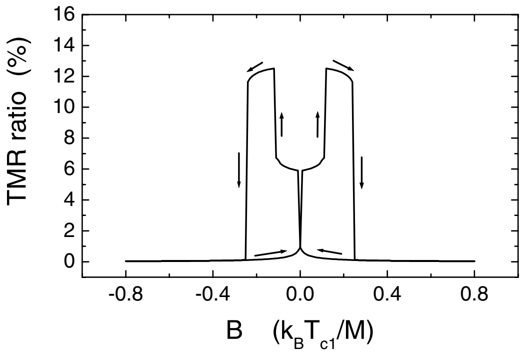

Figure 4. The TMR ratio as a function of the applied field in a hysteresis loop. The parameters are: $k_B T = 0.003$ eV, $E_F = 0.8$ eV, $U_0 = 4$ eV, $\lambda M = 0.1$ eV, $d = 2$ nm, and $U_2 = 0$. The Fermi wavenumber of the electrons with majority spin in the left FM layer k_{F0} is 1 nm^{-1}.

The TMR ratio may be optimized by tuning the structure of the system. In figure 5 we plot the TMR ratio as a function of thickness d in polarization configurations $\downarrow\uparrow\downarrow$ and $\downarrow\uparrow\uparrow$. The TMR ratio in configuration $\downarrow\uparrow\downarrow$ exhibits a maximum at a certain thickness. This behaviour is due to the quantum interference of electron waves scattered by two interfaces in this three-layer structure. One can see that on increasing the potential of the middle layer the peak height is almost unchanged but the corresponding thickness is enlarged, corresponding to the increase of the average de Broglie wavelength.

4. Summary

In summary, we investigated the hysteresis loop and the mechanism of the enhancement of the TMR ratio for three-layer structures. It is found that the quantum interference produced by two interfaces in such structures can lead to this enhancement for special thicknesses of the middle layer. The precondition for this enhancement is the existence of a range of external field under which the $\uparrow\downarrow\uparrow$ or $\downarrow\uparrow\downarrow$ configuration occurs. The optimal thickness of the middle layer depends on the average de Broglie wavelength. In a system with the middle layer made

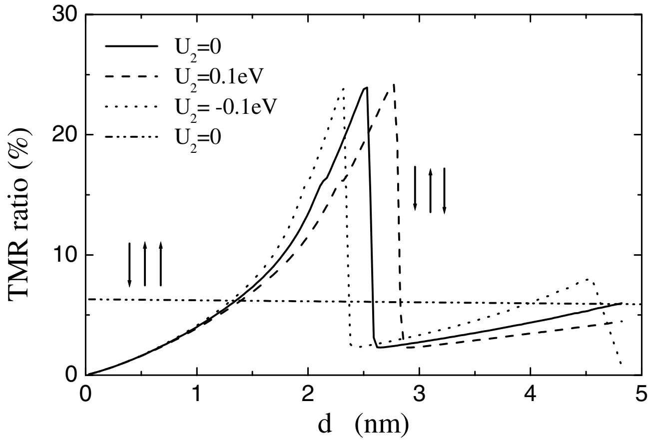

Figure 5. The TMR ratio as a function of the thickness of the middle layer for different values of U_2. The other parameters are the same as those for figure 4. The solid, dashed, and dotted lines are for configuration ↓↑↓, while the dot–dot–dashed line is for configuration ↓↑↑.

of insulator doped with FM ions, the enhancement of the TMR may not occur, because the magnetization in this layer is too small. This behaviour is observed in reference [4].

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