Spin-polarized tunneling and magnetoresistance in ferromagnet/insulator(semiconductor) single and double tunnel junctions subjected to an electric field

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Based on the two-band model, we present a transfer-matrix treatment of the tunnel conductance and magnetoresistance for tunneling through ferromagnet/insulator (semiconductor) single junctions and double junctions subject to a dc bias. Our results are qualitatively in agreement with the experimental measurements for the single junction. For the double junction, we find that there exists, spin-polarized resonant tunneling and giant tunnel magnetoresistance. The highest value of the magnetoresistance in a double junction can reach 90%. We anticipate that our results will stimulate some interest in experimental efforts in designing spin-polarized resonant-tunneling devices. [S0163-1829(97)00633-4]

I. INTRODUCTION

Since the early seventies, spin-polarized tunneling studies have been performed in order to access information about spin-dependent electronic states.[1,2] In recent years, with the progress in the research on magnetic multilayers, spin-polarized tunneling through ferromagnet/insulator (semiconductor)/ferromagnet (FM/I(S)/FM) junctions has received increasing attention.[3–6] This is mainly due to its widespread prospects of these multilayers for use as high-density, nonvolatile storage media or as field sensors.[4,8]

Recently, a few experiments[3–7] have been done to measure the tunnel conductance and magnetoresistance of the FM/I(S)/FM junctions. To explain the experimental results, two theories have been presented. A simple model proposed by Julliere[9] assumes that the spin is conserved in tunneling, and tunnel current is dependent on the density of states of the two electrodes. Another theory proposed by Slonczewski[10] analyzes the transmission of charge and spin currents through a rectangular barrier separating free-electron-like FM metals by means of a two-band model. These theories are successful in explaining some aspects of experimental phenomena for FM/I(S)/FM junctions. However, they neglect the effect of the electric field on the transmission coefficients and tunnel conductance; thus, other aspects of experimental phenomena, such as the decrease of the magnetoresistance with dc bias,[3] remain to be explained. As for the FM/I(S)/FM/I(S)/FM double junction, to our knowledge, neither experimental or theoretical investigation has been performed so far.

In this paper, we present a transfer-matrix treatment of the tunnel conductance and magnetoresistance for tunneling through FM/I(S)/FM and FM/I(S)/FM/I(S)/FM tunnel junctions under an electric field. Our treatment still relies on the free-electron model of the conduction electrons as in Ref. 10, for this model is relatively simple and has been adopted with success to study the spin-polarized tunneling between iron-group ferromagnetic metals and superconductors,[11] and the tunneling through metal-barrier-metal junctions.[14] Our goal is not limited to explaining experimental phenomena for the FM/I(S)/FM single junction, but we hope also to obtain the theoretical predictions for the FM/I(S)/FM/I(S)/FM double junction.

The organization of the rest of this paper is as follows. In Sec. II we describe the transfer-matrix approach of tunneling through single and double junctions. In Sec. III we present our calculated results on tunnel conductance and magnetoresistance. A brief summary is given in Sec. IV.

II. THEORY

We first consider the FM/I(S)/FM/I(S)/FM double junction in the presence of dc bias. The state densities of spin-up and spin-down electrons in a ferromagnet and the schematic potential are shown in Figs. 1(a) and 1(b), respectively. We assume that both the positive bias V_a and the electric field yielded by it across the barriers are constant. In a free-electron approximation of the spin polarized conduction electrons, the longitudinal part of the effective one-electron Hamiltonian may be written as

$$H=(-\hbar^2/2m_j^*)(d^2/dz^2)-F(z)+U(z)-\mathbf{h}(\mathbf{z})\cdot\sigma, \quad (1)$$

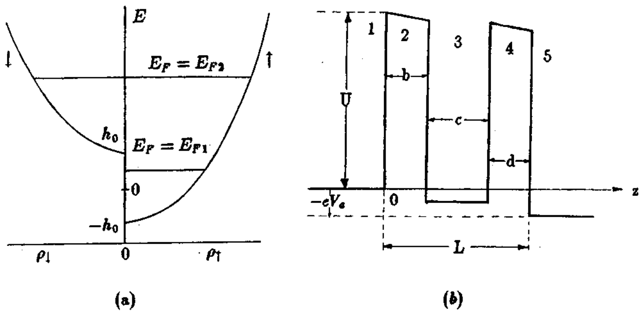

FIG. 1. (a) The state densities of spin-up ($\rho_\uparrow$) and spin-down ($\rho_\downarrow$) electrons, showing positions of Fermi energies $E_F = E_{F1}$ and $E_F = E_{F2}$ for the two-band model of a ferromagnet. (b) A schematic potential for the FM/I(S) double junction in an applied positive bias V_a. U is the barrier height and L the width of the double-barrier structure. b and d are, respectively, the width of the left and right barriers, c is the width of the middle ferromagnet, and V_a the applied constant bias voltage.

where

$$F(z) = \begin{cases} 0, & z<0, \\ eV_a z/(L-c), & 0<z<b, \\ eV_a b/(L-c), & b<z<b+c, \\ eV_a(z-c)/(L-c), & b+c<z<b+c+d, \\ eV_a, & z>b+c+d, \end{cases} \tag{2}$$

where m_j^*, $j=1\sim 5$, stands for the electron effective masses in the five regions labeled in Fig. 1(b). L, c, b, and d are the widths of the double-barrier structure, the middle ferromagnetic layer, and the left and right barrier, individually. $U(z)$ represents the barrier-potential profile, namely, $U(z)=U$ in barrier regions, $U(z)=0$ otherwise. $-\mathbf{h}(\mathbf{z})$ is the molecular field and σ is the conventional Pauli spin operator. We assume that $\mathbf{h}=\mathbf{0}$ inside the barriers and $|\mathbf{h}|=h_0$ within each ferromagnet. Although transverse momentum $\mathbf{k}_\parallel$ is omitted from the above notations, the summation[10] over $\mathbf{k}_\parallel$ is carried out in our calculations.

The Schrödingder equation for a biased barrier layer can be written by a simple coordinate transformation whose solutions are the Airy function $Ai[\rho(z)]$ and its complement $Bi[\rho(z)]$.[15] Considering all five regions of the double junction shown in Fig. 1(b), the general solution to the Schrödingder equation is thus

$$\psi_{j\sigma}(z) = \begin{cases} A_{1\sigma}e^{ik_{1\sigma}z}+B_{1\sigma}e^{-ik_{1\sigma}z}, & z<0, \\ A_{2\sigma}Ai[\rho_{2\sigma}(z)]+B_{2\sigma}Bi[\rho_{2\sigma}(z)], & 0<z<b, \\ A_{3\sigma}e^{ik_{3\sigma}z}+B_{3\sigma}e^{-ik_{3\sigma}z}, & b<z<b+c, \\ A_{4\sigma}Ai[\rho_{4\sigma}(z)]+B_{4\sigma}Bi[\rho_{4\sigma}(z)], & b+c<z<b+c+d, \\ A_{5\sigma}e^{ik_{5\sigma}z}+B_{5\sigma}e^{-ik_{5\sigma}z}, & z>b+c+d, \end{cases} \tag{3}$$

where

$$k_{1,\sigma} = \sqrt{2m_1^*(E+h_0\sigma)}/\hbar,$$

$$k_{3,\sigma} = \sqrt{2m_3^*(E+eV_a b/(L-c)+h_0\sigma)}/\hbar$$

or

$$k_{5,\sigma} = \sqrt{2m_5^*(E+eV_a+h_0\sigma)}/\hbar$$

is the electron momentum along the z axis. $\sigma=\pm 1$ corresponds to $\sigma=\uparrow,\downarrow$, respectively. $A_{j\sigma}$ and $B_{j\sigma}$ are constants to be determined, while

$$\rho_{j,\sigma}(z) = \frac{z}{\lambda_{0j}} + \beta_{0j,\sigma}, \tag{4}$$

$$\lambda_{0j} = \left[-\frac{(L-c)\hbar^2}{2m_j^* eV_a}\right]^{1/3}, \tag{5}$$

$$\beta_{0j,\sigma} = \begin{cases} \dfrac{(L-c)(E-U)}{eV_a\lambda_{0j}}, & j=2, \\ \dfrac{(L-c)[E-U-eV_a c/(L-c)]}{eV_a\lambda_{0j}}, & j=4. \end{cases} \tag{6}$$

A. The transmission coefficients

Upon applying the continuity of the wave function $\psi_{j\sigma}$ and its normalized derivative $(1/m_j^*)(d\psi_{j\sigma}/dz)$ at the boundaries, we can derive a matrix formula that connects the coefficients $A_{1\sigma}$ and $B_{1\sigma}$ with the coefficients $A_{5\sigma}$ and $B_{5\sigma}$ as follows:

$$\begin{bmatrix} A_{1\sigma} \\ B_{1\sigma} \end{bmatrix} = \mathbf{S}_{\text{total}} \begin{bmatrix} A_{5\sigma} \\ B_{5\sigma} \end{bmatrix}, \tag{7}$$

where

$$\mathbf{S}_{\text{total}}=\frac{k_{5,\sigma}}{k_{1,\sigma}}\begin{bmatrix} ik_{1,\sigma} & \dfrac{m_1^*}{\lambda_{02}m_2^*} \\ ik_{1,\sigma} & -\dfrac{m_1^*}{\lambda_{02}m_2^*}\end{bmatrix}\begin{bmatrix} Ai[\rho_{2,\sigma}(z=0)] & Bi[\rho_{2,\sigma}(z=0)] \\ Ai'[\rho_{2,\sigma}(z=0)] & Bi'[\rho_{2,\sigma}(z=0)]\end{bmatrix}\times\mathbf{ST}(z)$$
$$\times\begin{bmatrix} Ai[\rho_{4,\sigma}(z=b+c+d)] & Bi[\rho_{4,\sigma}(z=b+c+d)] \\ Ai'[\rho_{4,\sigma}(z=b+c+d)] & Bi'[\rho_{4,\sigma}(z=b+c+d)]\end{bmatrix}^{-1}\begin{bmatrix} ik_{5,\sigma} & \dfrac{m_1^*}{\lambda_{04}m_4^*} \\ ik_{5,\sigma} & -\dfrac{m_1^*}{\lambda_{04}m_4^*}\end{bmatrix}^{-1}\begin{bmatrix} e^{-ik_{5,\sigma}(b+c+d)} & 0 \\ 0 & e^{ik_{5,\sigma}(b+c+d)}\end{bmatrix}^{-1}, \tag{8}$$

$$\mathbf{ST}(z)=\mathbf{S}^{-1}[\rho_{2,\sigma}(z=b)]\times\mathbf{T}[k_3,c]\times\mathbf{S}[\rho_{4,\sigma}(z=b+c)], \tag{9}$$

$$\mathbf{S}[\rho_{j,\sigma}(z)]=\begin{bmatrix} Ai[\rho_{j,\sigma}(z)] & Bi[\rho_{j,\sigma}(z)] \\ Ai'[\rho_{j,\sigma}(z)] & Bi'[\rho_{j,\sigma}(z)]\end{bmatrix}, \tag{10}$$

$$\mathbf{T}(k_j,z)=\begin{bmatrix} \cos(k_j z) & -\dfrac{m_j^*}{k_j m_{(j+1)}^*\lambda_{(j+1)}}\sin(k_j z) \\ \dfrac{k_j m_{(j-1)}^*\lambda_{(j-1)}}{m_j^*}\sin(k_j z) & \dfrac{\lambda_{(j-1)}m_{(j-1)}^*}{\lambda_{(j+1)}m_{(j+1)}^*}\cos(k_j z)\end{bmatrix}. \tag{11}$$

Then, the transmission coefficient of the spin σ electron for the double-barrier structure shown in Fig. 1(b) is

$$P_\sigma=\frac{k_{5,\sigma}}{k_{1,\sigma}}\left|\frac{1}{S_{\text{total}}^{11}}\right|^2, \tag{12}$$

where $\mathbf{S}_{\text{total}}^{11}$ is the left-upper element of the matrix $\mathbf{S}_{\text{total}}$ defined in Eq. (7).

Here we would like to point out that although Eq. (12) is derived for the double junction, we can also extend it to the single junction and superlattice by modifying Eq. (8) and Eq. (9) as follows. Let $\mathbf{ST}(z)=1$, $\rho_{4\sigma}(z=b+c+d)$ be replaced by $\rho_{4\sigma}(z=b)$, m_4^* by m_2^*, λ_{04} by λ_{02}, k_5 by k_3, and $(b+c+d)$ by b in Eq. (8); then Eq. (12) gives the transmission coefficient of the spin σ electron tunneling through the single junction. Similarly, let n be the total number of barriers, l_k the distance from $z=0$ to the kth interface, c_m the width of the mth ferromagnetic layer in the FM/I(S) superlattice, $(L-c)$ replaced by $(L-\Sigma_{m=1}^{n-1}c_m)$, and c by c_m in Eqs. (5) and (6). Let $\rho_{4\sigma}(z=b+c+d)$ be replaced by $\rho_{2n,\sigma}(z=l_{2n-1})$, m_4^* by m_{2n}^*, λ_{04} by $\lambda_{0(2n)}$, k_5 by $k_{(2n+1)}$, $(b+c+d)$ by l_{2n-1} in Eq. (8) and let

$$\begin{aligned}\mathbf{ST}(z)=\mathbf{S}^{-1}&[\rho_{2,\sigma}(z=l_1)]\times\mathbf{T}[k_3,(l_2-l_1)]\\ &\times S^{-1}[\rho_{3,\sigma}(z=l_2)]\times\mathbf{S}[\rho_{4,\sigma}(z=l_2)]\\ &\times\cdots\times\cdots\mathbf{S}^{-1}[\rho_{2n-1,\sigma}(z=l_{2n-3})]\\ &\times\mathbf{T}[k_{(2n-1)},(l_{2n-2}-l_{2n-3})]\\ &\times\mathbf{S}[\rho_{2n,\sigma}(z=l_{2n-2})];\end{aligned} \tag{13}$$

then Eq. (12) gives the transmission coefficient of the spin σ electron tunneling through the FM/I(S) superlattice.

B. Tunnel conductance and magnetoresistance

The tunnel current per unit area for the double or single junctions at a given applied bias V_a can be calculated with the stationary-state (free-electron) model[16]

$$J_\sigma=\frac{em_j^*k_BT}{2\pi^2\hbar^3}\int_0^\infty P_\sigma(E,V)\times\ln\left\{\frac{1+\exp[(E_F^\sigma-E)/k_BT]}{1+\exp[(E_F^\sigma-E-eV_a)/k_BT]}\right\}dE, \tag{14}$$

where k_B is the Boltzmann constant, T the temperature, and E_F^σ the Fermi energy of the spin σ electron. According to the two-band model of Refs. 10 and 11, the tunnel conductance per unit area is $G=\Sigma_\sigma J_\sigma/V_a$. The tunnel magnetoresistance (TMR) can be expressed as

$$\text{TMR}=(G_{\uparrow\uparrow}-G_{\uparrow\downarrow})/G_{\uparrow\uparrow}, \tag{15}$$

where $G_{\uparrow\uparrow}$ and $G_{\uparrow\downarrow}$ represent the tunnel conductance of the FM/I(S) double or single junctions for parallel and alternately antiparallel alignments of the magnetizations in ferromagnetic layers, respectively.

III. NUMERICAL RESULTS AND DISCUSSION

Taking the Fe/Al_2O_3(MgO)/Fe single junction as an example, we calculate the tunnel conductance and magnetoresistance by making use of Eqs. (12) and (13). In the calculation E_F^σ and h_0 are taken according to Refs. 12, 13, and 2. The barrier heights are considered[4] above ~ 1 eV, and for convenience, we first neglect the difference of electron effective masses in barriers and ferromagnets, i.e., put[11] $m_j=m_e$.

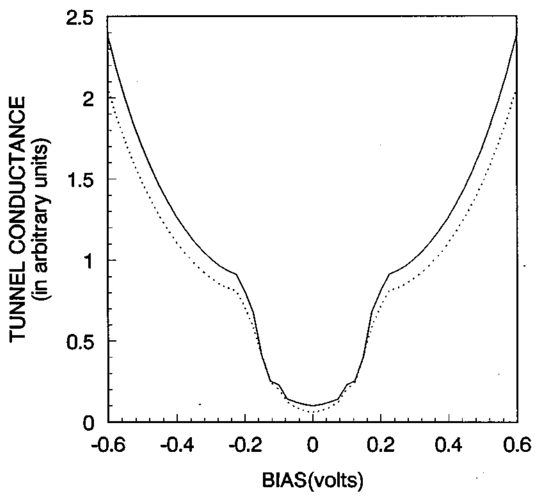

FIG. 2. Tunnel conductance as a function of dc bias for a Fe/I/Fe junction with $b=15$ Å and $U=1$ eV at $T=4.2$ K. The solid curve is for the two-band model and the dotted curve is only for spin-up electron.

Figures 2 and 3 show the tunnel conductance and magnetoresistance as a function of dc bias. At low bias the conductance varies only slightly with the bias, whereas at high bias a nearly parabolic dependence of conductance on the bias appears. The experimental result that TMR decreases with dc bias can be understood from our calculation; see Fig. 3. The reason is that with increasing dc bias the conductance of tunneling through the junction increase significantly; however, the difference between the conductance for parallel magnetization alignment from that for alternately antiparallel magnetization alignment increases only slightly. This leads to the decrease of TMR monotonously with increasing dc bias. Our results are qualitatively in agreement with the experimental measurements of Refs. 3 and 4. Quantitatively, however, there are some discrepancies between our results and experimental results. This may involve many factors, such as the surface roughness, spin-flip scattering, magnetic-

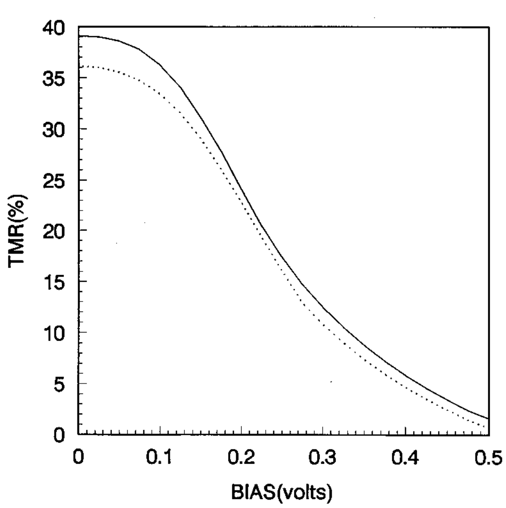

FIG. 3. TMR in the two-band model as a function of dc bias for a Fe/I/Fe junction with $b=10$ Å (solid curve) and $b=16$ Å (dotted curve) for $U=1.2$ eV at $T=4.2$ K.

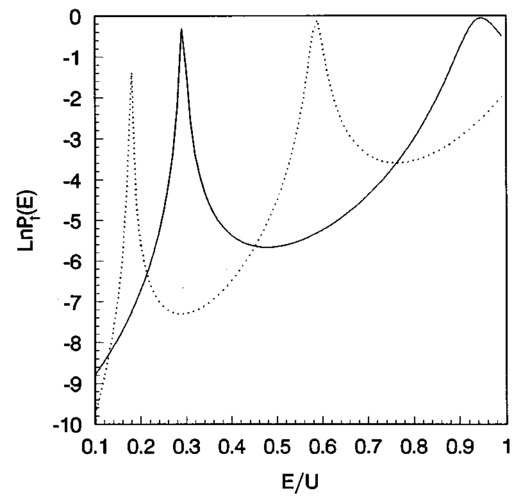

FIG. 4. Transmission coefficient ln $P(E)$ vs energy E for a Fe/I/Fe double junction ($b=d=5$ Å, $c=10$ Å) with $V_a=0.4$ V and $U=1.32$ eV. The solid curve is for parallel alignment of magnetizations in three ferromagnetic layers and the dotted curve is for the alignment where the magnetization in the middle ferromagnetic layer is antiparallel to that in the exterior ferromagnetic layers.

domain walls, electron-electron correlation, etc., which are neglected in our calculations. We also calculate the tunnel conductance and TMR of the Fe/Ge/Fe junction with the electron effective masses being taken as different values in Fe and Ge ($m_{\mathrm{Fe}}=m_e$ and $m_{\mathrm{Ge}}=0.082m_e$). We find that in this case the calculated results are similar to those shown in Figs. 2 and 3. These show that the two-band model, despite its simplicity, can indeed embody the main aspects of physics in tunnel junctions at low temperature. It should be pointed out that a numerical instability is encountered in some of our calculations at very low values of incident energy and electric field due to our use of exact Airy functions. Such an instability is overcome by using numerical analytical techniques and asymptotic forms of Airy functions.[15]

For double junctions, we consider two cases. In one case, the magnetizations in all three ferromagnetic layers are parallel, while in another case the magnetization in the middle ferromagnetic layer is antiparallel to that in the exterior ferromagnetic layers. The comparison of the transmission coefficients for spin-up electrons in these two cases are shown in Fig. 4. The results show that resonant tunneling exists in the FM/I(S) double junction as in the semiconductor double-barrier structure. However, the tunneling of either spin-up or spin-down electrons in the two cases are different from each other. Thus, we call such a type of tunneling ''spin polarized resonant tunneling.'' This leads to an essential distinction between the behaviors of tunnel conductance in double and single junctions. The tunnel conductance in the Fe/Ge double junction versus the dc bias is plotted in Fig. 5 and exhibits peaks of conductance under bias in contrast to the parabolically increasing of conductance with the bias in the single junction as shown in Fig. 2.

In Fig. 6, we plot the TMR as a function of the bias in the Fe/Ge double junction, for which the TMR varies with the electric field. In contrast, the TMR for the single junction decreases monotonously with the electric field as shown in Fig. 3. This kind of phenomenon is obviously caused by

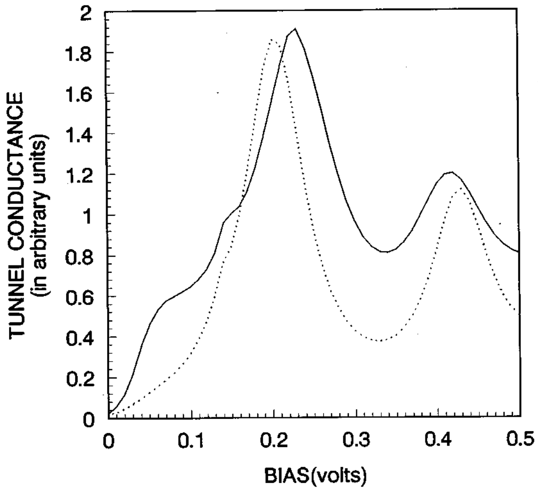

FIG. 5. Tunnel conductance (two-band model) for parallel alignment of magnetizations as a function of dc bias for a Fe/Ge/Fe/Ge/FM double junction ($b=d=5$ Å, $c=15$ Å) with $U=1.0$ eV (solid curve) and $U=1.2$ eV (dotted curve) at $T=8$ K.

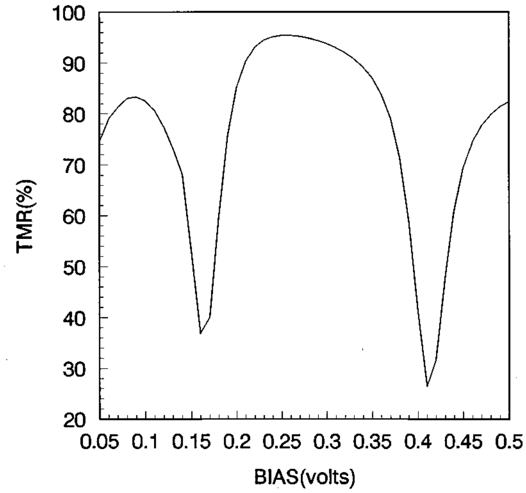

FIG. 6. TMR in the two-band model as a function of dc bias for a Fe/Ge/Fe/Ge/FM double junction ($b=d=5$ Å, $c=15$ Å) with $U=1.0$ eV at $T=8$ K.

spin-polarized resonant tunneling. The TMR under a certain bias can be improved greatly by using the double junction as compared with the single junction. The highest value of the TMR for the double junction can reach 90%.

IV. SUMMARY

Based on the two-band model, we presented a transfer-matrix treatment of the tunnel conductance and TMR for tunneling through FM/I(S) double and single junctions subjected to the electric field. For the single junction, our results are qualitatively in agreement with the experimental measurements; in particular, the monotonous decrease of TMR with bias can be explained from our results. For double junctions, we find that spin-polarized resonant tunneling and giant TMR exist. We hope that our results can stimulate interest in experimental efforts in designing spin-polarized resonant tunneling devices.

ACKNOWLEDGMENT

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