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2003 J. Phys.: Condens. Matter 15 4841

(http://iopscience.iop.org/0953-8984/15/27/315)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **15** (2003) 4841–4850 PII: S0953-8984(03)61939-9

Enhanced spin injection efficiency in ferromagnet/semiconductor tunnel junctions

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Received 9 April 2003
Published 27 June 2003
Online at stacks.iop.org/JPhysCM/15/4841

Abstract

Within the ballistic transport picture, we have investigated the spin-polarized transport properties of a ferromagnetic metal/two-dimensional semiconductor (FM/SM) hybrid junction and an FM/FM/SM structure using quantum tunnelling theory. Our calculations indicate explicitly that the low spin injection efficiency (SIE) from an FM into an SM, compared with a ferromagnet/normal metal junction, originates from the mismatch of electron densities in the FM and SM. To enhance the SIE from an FM into an SM, we introduce another FM film between them to form FM/FM/SM double tunnel junctions, in which the quantum interference effect will lead to the current polarization exhibiting periodically oscillating behaviour, with a variation according to the thickness of the middle FM film and/or its exchange energy strength. Our results show that, for some suitable values of these parameters, the SIE can reach a very high level, which can also be affected by the electron density in the SM electrode.

1. Introduction

In recent years there has been much theoretical and experimental work in the so-called spintronics field [1–3], in which the degrees of freedom of both electronic spin and charge are exploited. Spin-based devices [4] have advantages over charge-based devices and numerous potential applications, especially in the information technology industry. The efficient injection of the spin-polarized electrons into a semiconductor (SM) is one of the key issues for incorporating electron spins into well developed SM technology. The injection of spin-polarized carriers from a ferromagnetic SM into a nonmagnetic SM [5–7] has been achieved successfully with an efficiency of ∼90%. Spin injection from a ferromagnetic metal (FM) into a SM is more attractive, because FMs such as Fe and Co have a relatively high Curie temperature, which makes them indispensable for room-temperature devices. However, at present the spin injection efficiency (SIE) from an FM into an SM is very low and, moreover, there is also much debate about it [8].

As pointed out by Schmidt *et al* [9], the basic obstacle to spin-polarized electron injection from an FM into an SM in the diffusive system results from the mismatch in their conductivities. Many authors [10–12] have shown that this kind of conductivity mismatch could be circumvented by introducing a tunnel barrier (I) between them, which can induce spin-dependent tunnelling conductance. Currently, it is not yet very clear that the tunnel barrier is indeed necessary for spin injection from an FM into an SM [13, 14]. Kirczenow [15] predicted theoretically that certain atomically ordered interfaces between an FM and an SM should act as ideal spin filters, i.e. only the majority-spin or minority-spin electrons can tunnel through the FM/SM junction. Considering complex electronic structures of FM and SM materials as well as complex properties of the interface, Matsuyama *et al* [16] and Mavropoulos *et al* [17] employed an *ab initio* method to calculate the SIE in Fe/InAs(GaAs) junctions and Fe/InAs(GaAs)/Fe double junctions, respectively, and found that SIE can achieve 100%. However, these results do not agree well with recent observations from experiments [18–21]. With a tunnel barrier, the magnitude of the SIE is about 10% in the present experimental observations [18–20], e.g. a Schottky barrier formed at the Fe/AlGaAs interface can make the efficiency of spin injection $\sim$13% in this tunnel junction [21].

Based on the assumption that the system's conductance is determined by the density of states of the SM at its Fermi energy, Grundler [22] and Hu and Matsuyama [23], independently, employed Landauer–Büttiker formalism to investigate ballistic transport in the FM/SM hybrid junction. They found a low SIE that is consistent with the above experimental results. In the present work, we use quantum tunnelling theory [24, 25] to study the same FM/SM heterojunction and find that the electrical conductance of the FM/SM heterojunction does not depend strongly on the spin-polarized Fermi velocity in the FM electrode, which is different to the FM/normal metal (NM) junction. The extremely low electron density of an SM compared to that of an FM as well as the conservation rules of the interface tunnelling process cause the low efficiency of spin injection from the FM into the SM. When a tunnel barrier is introduced in this FM/SM junction, the transmission of the minority-spin electron with lower kinetic energy decreases greatly, making the SIE increase. (In this study we assume spin-down as the minority spin.)

In order to increase the SIE from the FM to the SM, we propose the introduction of another FM layer into the system and study the new FM/FM/SM double junctions. The left-hand FM electrode of the FM/FM/SM junction is a source of spin injection electrons, while the middle FM film operates as a resonant device to tune the tunnelling current. The quantum resonant tunnelling has recently been realized experimentally in FM/NM/FM double junctions [26]. Our analysis and calculated results show that the resonant tunnelling in an FM/FM/SM structure does make the SIE—which is also affected by the electron density in the SM layer—reach a very high level for some suitable parameters.

The rest of this paper is organized as follows. In section 2, a simple two-dimensional quantum tunnelling model is established as well as the formalism of tunnelling conductance. The real physical origin of the low efficiency of spin injection from an FM into an SM is obtained in section 3 by studying the FM/SM single junction. In section 4, the FM/FM/SM double junctions are investigated in order to enhance current polarization. Conclusions are drawn in section 5.

2. Model

We consider first a single FM/SM heterojunction with its interface located at $x = 0$. When an external voltage is applied, an electric current flows along x-direction. For the FM electrode, the energy dispersion is taken to be of simplified parabolic form and the spin polarization is described by the Stoner model with an exchange splitting energy Δ. Meanwhile, for the SM electrode, here we neglect the so-called Rashba spin–orbit coupling term [27] because it may not lead to the splitting of two spin subbands [28, 29] and its order is much lower than Fermi energy (E_F). Using the free-electron approximation, the Hamiltonian for the FM/I/SM junction reads

$$\mathcal{H} = \frac{-\hbar^2}{2m(x)}\nabla^2 - \theta(-x)\boldsymbol{h}\cdot\boldsymbol{\sigma} + U\delta(x), \tag{1}$$

where: $m(x)$ is the effective electron mass $m(x) = m_\mathrm{e}$ in the FM for $x < 0$ and $m(x) = m_\mathrm{s}$ in the SM for $x > 0$; $\boldsymbol{h}$ is the internal molecular field of the FM and $\boldsymbol{\sigma}$ denotes the Pauli spin operator; and $\theta(x)$ is the step function. The thin tunnel barrier is described by a δ-type potential, which does not lose generality, and U is related to the barrier's width and height.

When a small bias is applied to this FM/SM single junction, only the electrons near the Fermi energy (E_F) contribute greatly to the net tunnel current. We consider not only the electrons in the FM with their momentum direction perpendicular to the interface, but also those electrons with their momentum direction angled to the normal direction of the interface, i.e. both perpendicular and oblique incidences of electrons from the FM into the SM are taken into account on the same footing. According to the requirements of ballistic transport, when an electron passes through an interface its energy and momentum parallel to the interface ($k^{\parallel}_{\mathrm{F},\sigma}$) must be conserved. We define the angle of incidence of the electron, ϕ, as

$$k^{x}_{\mathrm{F},\sigma} = k_{\mathrm{F},\sigma}\cos\phi, \qquad k^{\parallel}_{\mathrm{F},\sigma} = k_{\mathrm{F},\sigma}\sin\phi. \tag{2}$$

For the SM, the Fermi momentum can be expressed simply as $k_\mathrm{sm} = \sqrt{2\pi n_\mathrm{D}}$ (n_D denotes the electron density in SM), assuming parabolic subband dispersion, which is spin independent. Using the standard quantum mechanical method, for the FM/SM single junction the spin-dependent transmission for each electron with incident momentum $k^{x}_{\mathrm{F},\sigma}$ is obtained as

$$T_\sigma = \frac{4\beta_\sigma}{(1+\beta_\sigma)^2 + Z_\sigma^2}, \tag{3}$$

where $\beta_\sigma = v^{x}_{\mathrm{sm}}/v^{x}_{\mathrm{F},\sigma}$ and $Z_\sigma = 2U/\hbar v^{x}_{\mathrm{F},\sigma}$, and $v^{x}_{\mathrm{F},\sigma}$ and v^{x}_{sm} denote the Fermi velocity of the electron along the x-direction in the FM and SM electrodes, respectively. For small biases at low temperatures, the electrical conductance of the system can be expressed as [25, 31]

$$G_\sigma = \frac{e^2 k_{\mathrm{F},\sigma}}{h\pi}\int_0^{\phi^\mathrm{C}_\sigma} \mathrm{d}\phi\, T_\sigma \cos\phi, \tag{4}$$

where ϕ^C_σ is the critical angle of incidence of the electron with spin σ in the FM electrode. This angle guarantees that all momenta appearing in the integral are real variables. Due to $k_\mathrm{sm} \ll k_{\mathrm{F},\sigma}$, which comes from the fact that the electron density of an SM is much lower than that of a metal, the critical angle of incidence can therefore be approximated as $\phi^\mathrm{C}_\sigma = \sin^{-1}(k_\mathrm{sm}/k_{\mathrm{F},\sigma}) \simeq (k_\mathrm{sm}/k_{\mathrm{F},\sigma})$.

Since $\phi^\mathrm{C}_\sigma \sim 0$, most electrons at the Fermi energy in the FM electrode do not contribute to the tunnel current and only very few electrons with angles of incidence smaller than ϕ^C_σ can take part in the current process. Because $\phi^\mathrm{C}_\uparrow < \phi^\mathrm{C}_\downarrow$, the influence of the spin-polarized density of states at the Fermi energy of the FM on the tunnel current is weakened. This may cause the low efficiency of spin injection from the FM into SM, which is defined as the current polarization:

$$P = \frac{G_\uparrow - G_\downarrow}{G_\uparrow + G_\downarrow}. \tag{5}$$

3. FM/SM single junction

It is well known that spin-polarized current can easily be achieved in FM/NM heterojunctions [32]. We will study the current polarization, P, of the FM/SM junction in comparison to that of the FM/NM junction using the above equations, as they are general for all heterojunctions. We take the metal Fe as the FM electrode and InAs as the SM. The Fermi momentum of the majority spin and the minority spin of Fe are chosen as $k_{\mathrm{F},\uparrow} = 1.05 \times 10^8\ \mathrm{cm}^{-1}$ and $k_{\mathrm{F},\downarrow} = 0.44 \times 10^8\ \mathrm{cm}^{-1}$ [22, 30]. Electron densities in the InAs electrode are typically in the range $1.0 \times 10^{12}\ \mathrm{cm}^{-2} < n_\mathrm{D} < 3.0 \times 10^{12}\ \mathrm{cm}^{-2}$. We choose the effective mass of the SM to be $m_\mathrm{s} = 0.036\ m_\mathrm{e}$. There is a difference between d-electrons in FMs and s-electrons in NMs. In an FM the d-electron has a large effective mass and a small $E_\mathrm{F} - E_{\mathrm{bottom}}$, while in an NM the s-electron has a small effective mass and a large $E_\mathrm{F} - E_{\mathrm{bottom}}$. Since $k_\mathrm{F}^2 = 2m_{\mathrm{eff}}[E_\mathrm{F} - E_{\mathrm{bottom}}]$, the Fermi momenta in the FM and NM may be of the same order of magnitude. For convenience, the parameters used in our calculation for the NM are the same as those of the FM except the spin polarization, which affects k_F in the FM but is nil in the NM. The density of electrons in the SM is taken to be $n_\mathrm{D} = 1.5 \times 10^{12}\ \mathrm{cm}^{-2}$.

We first consider the case of tunnel barrier $U = 0$ at the interface and calculate the current polarization of the structure. In figure 1 the results are plotted as a function of the dimensionless polarization in the FM, defined as the exchange splitting energy Δ normalized by the E_F of the FM. The plots show the current polarization of both FM/NM and FM/SM junctions with variation of spin polarization of the FM. The current polarization, P, of the FM/NM junction increases greatly with increasing spin polarization of the FM [32]. This can be interpreted as follows. Since, in equation (4), $k_{\mathrm{F},\uparrow} > k_{\mathrm{F},\downarrow}$ and $\phi_\sigma^\mathrm{C} \sim \pi/2$ (resulting in the Fermi momenta in the FM and the NM having the same order of magnitude), $G_\uparrow$ is always larger than $G_\downarrow$ and the difference between them increases when the kinetic energy of the spin-down electron decreases continuously. While, for the FM/SM junction, the current polarization, P, keeps very low and varies little, until the spin polarization Δ/E_F in the FM arrives near to 100%, when P increases significantly. This feature agrees with the result from Landauer–Büttiker formalism [22]. This is not caused by the transmission coefficients T_σ in equation (4), because the Fermi velocity of the electron in the NM has the same order of magnitude as that in the SM. Hence, this feature can only result from the critical angle of incidence ϕ_σ^C. As discussed above, $k_{\mathrm{sm}} \ll k_{\mathrm{F},\sigma}$ and $\phi_\sigma^\mathrm{C} \sim 0$ for the electron density in the SM, which are is much less than those in the FM, so equation (4) can be approximated as

$$G_\sigma = \frac{e^2 k_{\mathrm{sm}}}{h\pi} T_\sigma \bigg|_{\phi=0}. \tag{6}$$

This formalism has a similar formation to that of Landauer–Büttiker theory [22]. Unlike in the FM/NM junction, the electrical conductance of the FM/SM heterojunction is related to unpolarized Fermi wavevector k_{sm} in the SM. Consequently, the advantage of the spin-polarized density of states at the Fermi energy of the FM (which causes current polarization in the FM/NM junction) vanishes in the FM/SM junction. From the above analysis, we may conclude that the real physical origin of the low SIE from the FM into the SM is due to the electron density in the SM being much less than that in the FM, as well as the conservation rules of the quantum tunnelling process in ballistic transport.

To illustrate the effect of the electron density of the SM, we plot in figure 2 the normalized conductance of the FM and the current polarization against the electron density of the SM n_D. Figure 2(a) shows the variation of the conductances as n_D changes, with Fe being the FM material ($\Delta/E_\mathrm{F} = 0.82$). The conductances due to the electrons of both spin orientations increase as n_D increases. However, $G_\uparrow$ surpasses $G_\downarrow$ at a crossing point. Figure 2(b) plots

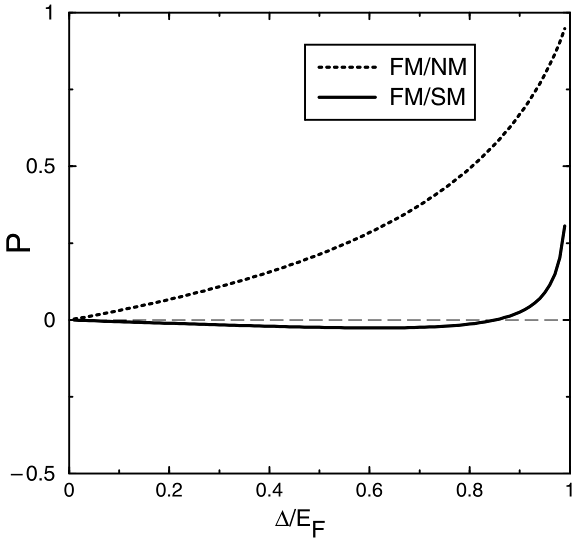

Figure 1. The current polarization, P, in the FM/NM and FM/SM heterojunctions as a function of the spin polarization, Δ/E_{F}, of the FM electrode. E_{F} is the Fermi energy in FM. Parameters are described in the text.

the dependence of two current polarization levels on n_{D} when Fe and FeNi ($\Delta/E_{\mathrm{F}} = 0.4$) are the FM materials, respectively. When n_{D} increases, $\phi_{\sigma}^{\mathrm{C}}$ becomes larger and more electrons contribute to the tunnelling current. Thus, the current polarization may transfer from a negative value [16] to a positive value because of $T_{\uparrow} > T_{\downarrow}$. The transition point of the solid curve (Fe as the FM) in figure 2(b), at which the current polarization changes sign, corresponds to the crossing point in figure 2(a). Also, from figure 2, we can see that the transition point for each case falls into the range of electron densities, n_{D}, in the popular SM materials that are most commonly investigated in this area at present ($1 - 4 \times 10^{12}$ cm^{-2}). In other words, the spin injection processes in these FM/SM junctions are all around the transition points at which the magnitude of the polarization is near to zero. So, the SIE from FMs into SMs appears to be very low at present.

As a tunnel barrier is introduced, the transmission coefficient of the spin-down electron (minority) will decrease greatly because its kinetic energy is lower than that of the spin-up electron (majority). Figure 3 illustrates the influence of the barrier strength, defined as $Z_{\uparrow} = 2U/\hbar k_{\mathrm{F},\uparrow}$, on the electrical conductance and the current polarization. It is shown in figure 3(a) that $G_{\downarrow}$ decreases more rapidly than $G_{\uparrow}$ when the tunnel barrier strength grows. The positive current polarization at zero barrier increases monotonically with growth of the tunnel barrier strength. However, the magnitude of P at a smaller n_{D} (the solid curve, $P < 0$) will decrease first, until P changes its sign, then the magnitude of this positive current polarization is enhanced, as shown figure 3(b). For a larger electron density, n_{D}, in the SM, increasing the tunnel barrier strength will result in growth in the magnitude of the FM/SM junction's current polarization. We wish to point out that our analysis above is based on ballistic transport, and the resistivity of the SM is not taken into account in our free-electron model [22]. If diffusive scattering is considered at the interface, then the transmission and conductance of the FM/SM junction in figure 2 will decrease. Moreover, SIE will also decrease because the spin-flip effect may occur.

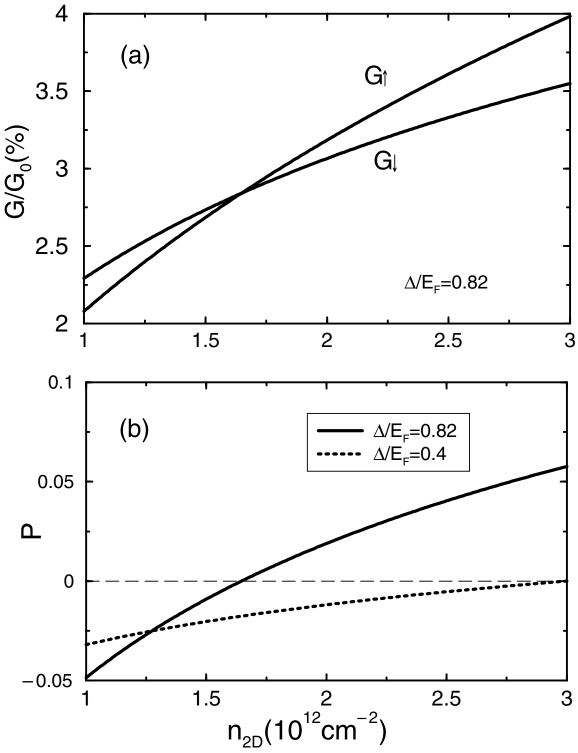

Figure 2. (a) The electrical conductance, G/G_0, for metal Fe as the FM electrode and (b) current polarization, P, of the FM/SM junction for two different FMs, $\Delta/E_\mathrm{F} = 0.82$ and 0.4, versus the electron density of the SM. Here, $G_0 = \frac{e^2 k_{\mathrm{F},\uparrow}}{h\pi}$ and other parameters are described in the text.

4. FM/FM/SM double junctions

Although a strong tunnel barrier can enhance the current polarization in the FM/I/SM junction, it can also greatly decrease the electrical conductance. This may lead to difficulty in experimental observation. Recently, the use of quantum resonant tunnelling in the FM/NM/FM heterojunctions [26] to achieve tunnel magneto-resistance (TMR) effect has been reported, and the results are encouraging. Here we propose the introduction of another FM film in the FM/SM single junction to form FM/FM/SM double junctions and utilize a quantum-interference effect in the middle FM film to achieve a high efficiency of spin injection from the FM into the SM. For convenience, we denote the left-hand FM and the middle FM as FM1 and FM2 and their exchange splitting energies as Δ_1 and Δ_2, respectively. Further, we assume that the magnetizations of the two FMs are parallel.

In this new structure, equation (4) is still valid for describing the electrical conductance of the system, but the expression of the spin-dependent transmission T_σ is different from equation (3). We can calculate numerically the spin-dependent electrical conductance as a function of thickness, (L), of the FM2 film, in which the multi-reflection would lead to resonant tunnelling transmission. Thus, the transmission coefficient T_σ exhibits oscillating behaviour, as does the electrical conductance G_σ. Their periods can be expressed approximately as $L_\sigma = \pi/k_{\mathrm{F},\sigma}^{(2)}$, since the critical angle ϕ_σ^C is very small, where $k_{\mathrm{F},\sigma}^{(2)}$ is the Fermi wavevector of FM2. Due to the presence of the exchange energy of FM2, $k_{\mathrm{F},\uparrow}^{(2)} \neq k_{\mathrm{F},\downarrow}^{(2)}$, the electrical conductances

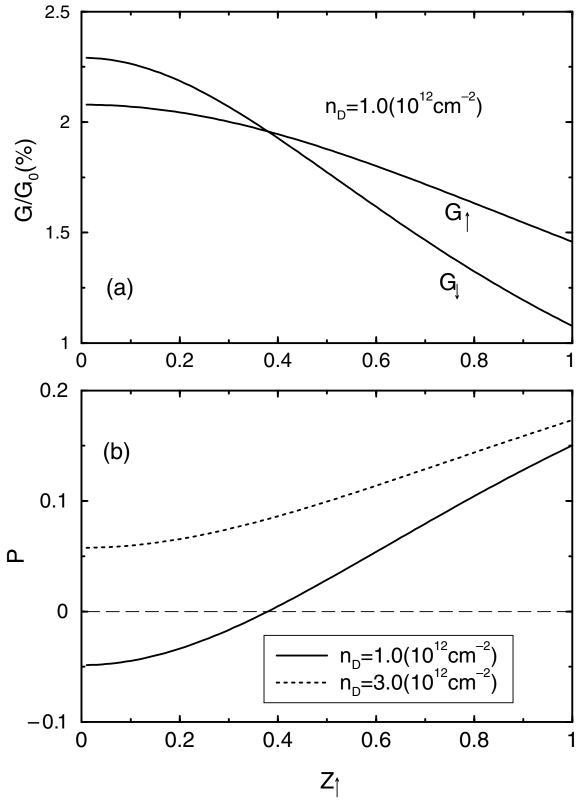

Figure 3. (a) The electrical conductance G/G_0 and (b) current polarization P as a function of barrier strength $Z_\uparrow = 2U/\hbar k_{F,\uparrow}$. The spin polarization of the FM electrode is $\Delta/E_F = 0.82$.

$G_\uparrow$ and $G_\downarrow$ have different oscillation periods, so the current polarization may achieve a rather high level for some suitable thickness L, as shown in figure 4. This characterization is the same as the TMR effect in the FM/NM/FM double tunnel junctions [33, 34], in which large TMR could be achieved because of the resonant tunnelling transmission of electronic waves in the NM film. Hence, the resonant states in the enhancement of TMR or SIE in these double tunnelling junctions play a similar and significant role.

The oscillating period of $G_\uparrow$ is different to that of $G_\downarrow$, so their superposition will cause a long- and a short-periodic oscillation of the current polarization P in figure 4. Even a NM ($\Delta_1 = 0$) replacing FM1 can also lead to current polarization, because of the presence of the FM2 film. Enlarging the exchange energy (Δ_1) of FM1, the overall profile of P stays almost invariant, whereas its amplitude increases greatly (solid curve), i.e. an increment in the spin-polarized level in FM1 will raise the SIE from FM1 into the SM. For $L = 0$, our model becomes an FM/I/SM single tunnel junction [31], and an NM ($\Delta_1 = 0$) as FM1 would result in a vanishing current polarization (dashed curve). When another FM metal (FM2) is interposed into such a single junction ($L \neq 0$), for some suitable thicknesses the current polarization would increase greatly comparison to that for $L = 0$.

Although the optimum current polarization P in figure 4 may be obtained by tuning the thickness of FM2, it oscillates quickly with an increase in L. This may cause the maximum of P to be difficult to find in experiment. However, in our model the oscillating periods of $G_\uparrow$

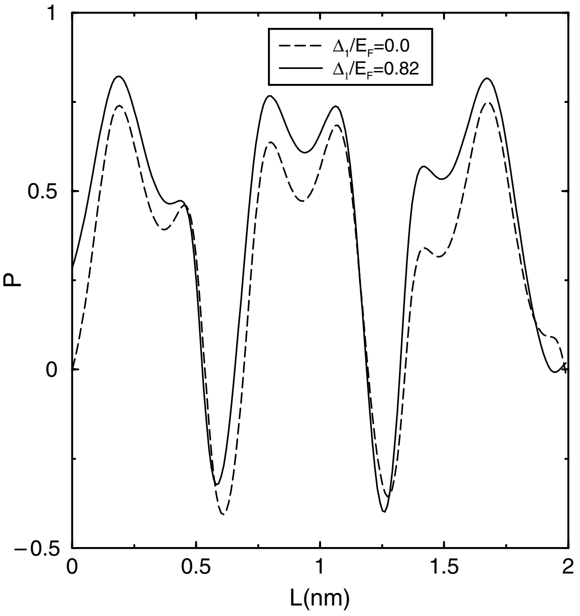

Figure 4. The current polarization, P, as a function of the thickness, L, of the middle FM film in FM/FM/SM double junctions for two different spin polarizations in FM1: $\Delta_1/E_F = 0.0$ and $\Delta_1/E_F = 0.82$. Metal Fe is taken as FM2 and $\Delta_2/E_F = 0.82$ The density of electrons in the SM is $n_D = 2.2 \times 10^{12}$ cm^{-2} and the tunnel barrier is $Z_\uparrow = 1.0$.

and $G_\downarrow$ depend on not only the thickness L but also the exchange energy Δ_2 of the FM2 layer. Thus, fixing the thickness L and varying the exchange energy (Δ_2) of FM2, the oscillating behaviour of the current polarization P should also appear. This is actually true, as shown in figure 5, which plots the current polarization as a function of the normalized spin polarization of FM2, where L is fixed as 15 Å, which is much less than the spin-flipping length in the FM. With increasing Δ_2, P will alternate its sign and take its peaks at some suitable values of Δ_2. Since the overall trend of minority-spin conductance $G_\downarrow$ decreases with increasing Δ_2, the maximum of the positive current polarization P will keep going up. Compared with figure 1, increasing the spin polarization of FM2 will greatly increase the current polarization, due to quantum resonant tunnelling. If $\Delta_2 > E_F$, FM2 would be a half-metal, such that it becomes a potential well for spin-up (majority-spin) electrons and a rectangle barrier for spin-down (minority-spin) electrons. The transmission coefficient of a spin-up electron is much larger than that of a spin-down electron, which leads to the high level of current polarization (even 100%) [35]. From figure 5, it is suggested that, for a non-half-metal, the high level of current polarization in FM/FM/SM junctions can be achieved by tuning the magnitude of FM2's exchange energy (Δ_2).

It follows from figure 5 that the electron density of the SM, n_D, can affect the SIE. The critical angle of incidence, ϕ_σ^C, of electrons in FM1 is determined by n_D. The larger n_D widens ϕ_σ^C, so the tunnel conductance G_σ increases greatly, whereas the SIE decreases. In these FM/FM/SM junctions, the high level of current polarization originates from the quantum interference effect. Usually, quantum interference devices have to be single-mode in order to obtain large effects, because different phase shifts exist in different modes. The larger ϕ_σ^C will introduce more modes and the quantum interference effect tends to be washed out, so the current polarization could decrease [4].

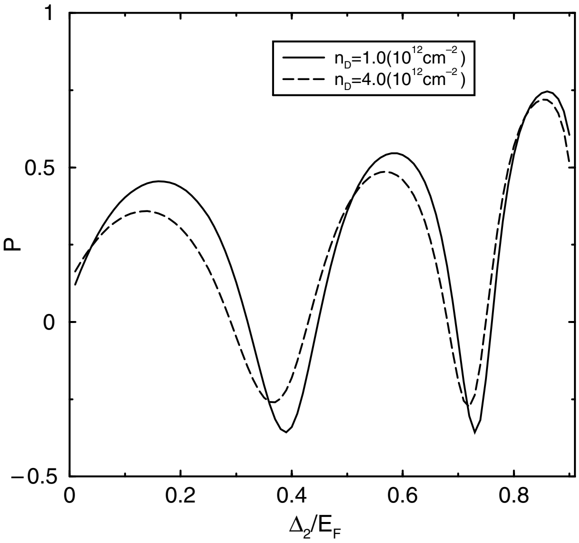

Figure 5. The current polarization, P, as a function of the exchange energy strength Δ_2/E_F of FM2. The dotted curve and the solid curve respectively denote two different electron densities of SM: $n_D = 1.0 \times 10^{12}$ and 4.0×10^{12} cm^{-2}. Here, $\Delta_1/E_F = 0.82$ and $L = 15$ Å.

5. Conclusion

In summary, we have studied the ballistic transport properties of the FM/SM and FM/FM/SM heterojunctions using quantum tunnelling theory. Compared with the FM/NM heterojunction, the low efficiency for spin injection from a FM into a SM originates from the mismatch in their electron densities. In the FM1/FM2/SM double junctions, a high level of current polarization can be achieved at some suitable thickness L and/or exchange energy Δ_2 of the FM2 layer. It is also shown that the electron density of the SM can alter the SIE.

Acknowledgments

This work was supported by the Australian Research Council under Project LX0347471. D Y Xing is grateful for support from the National Natural Science Foundation of China under Grant No 10174011 and the state key programmes for Basic Research of China.

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