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Spin-Polarization in Quasi-Magnetic Tunnel Junctions *

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Spin polarization in ferromagnetic metal/insulator/spin-filter barrier/nonmagnetic metal, referred to as quasi-magnetic tunnel junctions, is studied within the free-electron model. Our results show that large positive or negative spin-polarization can be obtained at high bias in quasi-magnetic tunnel junctions, and within large bias variation regions, the degree of spin-polarization can be linearly tuned by bias. These linear variation regions of spin-polarization with bias are influenced by the barrier thicknesses, barrier heights and molecular fields in the spin-filter (SF) layer. Among them, the variations of thickness and heights of the insulating and SF barrier layers have influence on the value of spin-polarization and the linear variation regions of spin-polarization with bias. However, the variations of molecular field in the SF layer only have influence on the values of the spin-polarization and the influences on the linear variation regions of spin-polarization with bias are slight.

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The effectiveness of spin-dependent electronic devices, which have many potential applications on magnetic memories and sensors, is related to the highly spin-polarized electric currents.[1,2] The simplest and most widely available methods of generating highly spin-polarized electric currents are through magnetic tunnel junctions (MTJs).[2] Traditional MTJs are constructed by the two layer ferromagnetic metal electrodes (FM) and a thin insulating layer (I) acting as a tunnel barrier (FM/I/FM), and can produce only partial spin polarization in the transport currents as the limitation spin dependent density of states in FM electrodes. For improving the TMR and the spin-polarization in MTJs, many methods are suggested, and among them, the MTJs using MgO as the nonmagnetic insulating barrier capture the attention as the symmetry filtering effects induced by their crystallographic configurations. Taking advantage of the coherent wave-function symmetry filtering effect, the large TMR and spin-polarization have been predicted firstly by the theoretical works[3] and followed by the experimental works.[4] Recent works further show that MgO-based magnetic tunneling junctions as its large TMR and low resistance would have the most promising ingredient for magnetic random access memories (MRAM) and the other spin devices.[5] As the free-electron treatment is no longer valid in MgO barriers, the TMR ratio has no relation with spin polarization in epitaxial MgO-based MTJs based on the first-principles calculation.[3] This feature is different from the amorphous AlO-based MTJs in which higher spin polarization shows a higher TMR ratio based on the Julliere model.[6] Alternative systems proposed for overcoming the shortcomings in conventional MTJs utilize the ferromagnetic insulator materials such as EuO, EuS and $CoFe_2O_4$ as the tunneling barriers.[2,7,8] The ferromagnetic insulator tunnel barriers have spin-filter (SF) effects that only one spin orientation electrons can easily tunnel through the barrier and the other orientation electrons can be effectively filtered out as the evanescence of the corresponding spin-dependent wave function in the barrier. Due to the high efficiency of spin filter tunnel barriers, extremely large spin-polarization and tunnel magnetoresistance (TMR) are expected.[9−15] The main types of spin filter magnetic junctions are single and double junctions. The example for double spin-filter junctions are the MTJs with two EuS spin filter barriers and have a form as NM/SF/I/SF/NM, where NM is a nonmagnetic metal electrode. According to the data demonstrated in recent experiments, TMR of about 33% was obtained.[14] The example for single spin-filter junction is the quasi-magnetic tunnel junctions (QMTJs) with one EuS barriers suggested by Refs. [9,10] that have a form as FM/I/SF/NM. The experimental and theoretical results indicated that well-defined and large TMR of about 55% responses have been realized in QMTJs utilizing different SF materials.[10,16] The main characteristics of spin-filter junctions are their bias dependences of TMR, which are quite different from the conventional MTJs. In conventional MTJs, the TMR decreases with increasing bias. However, in the spin-filter junctions, the TMR increases with the increasing bias. This feature makes spin-filter junctions that have potential applications in the devices worked at higher voltages. However, the exiting theoretical and experimental researches mainly focus on the TMR effect, and the spin-polarization has been mostly overlooked. In this Letter, based on the exiting experimental results, the spin-polarization of the transport current in FM/I/SF/NM quasi-spin filter tunnel junctions (QMTJs) is studied theoretically. The dependences of spin-polarization on bias with various barrier thicknesses, barrier heights and

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molecular fields are investigated. Our calculation results should be of concern for researchers who work on the spin filter junctions.

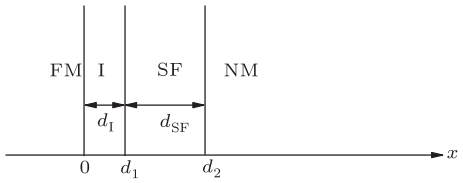

Fig. 1. A schematic diagram of FM/I/SF/NM quasi-spin filter tunnel junctions.

Based on the Slonczewski free electron model and Julliere's tunneling probability method,[6,17] the Hamiltonian with QMTJs is given by

$$\hat{H} = -\frac{\hbar^2}{2m^*}\nabla^2 + U(x). \tag{1}$$

$$U(x) = \begin{cases} h_{\rm FM}\sigma_z, & x < 0, \\ U_{\rm I} - \frac{evx}{d_{\rm I}+d_{\rm F}}, & 0 < x < d_1, \\ U_{\rm F} - \frac{evx}{d_{\rm I}+d_{\rm F}} - h_{\rm F}\sigma_z, & d_1 < x < d_2, \\ 0, & x > d_2, \end{cases} \tag{2}$$

where m^* is the electron effective mass, σ_z $(= \pm 1$, corresponding to the $\uparrow, \downarrow$ spin electrons, respectively) denotes the Pauli spin matrices, $h_{\rm FM}$ and $h_{\rm F}$ are the exchange splitting energy in the ferromagnetic electrode and the spin-filter barrier, $U_{\rm I}$ and $U_{\rm F}$ are the potentials in the I and spin-filter barrier, respectively. From the above Hamiltonian, we can see that the effective magnetic field (molecular field) makes the barrier height split via the Zeeman effect. Therefore, the barrier height experienced by a tunneling electron depends on its spin orientation.

The bias dependence of the spin-polarization of conduction electrons in the quasi-spin filter tunnel junctions can be obtained by the multi-step rectangular approximation method for treating electron transportation in nonmagnetic tunnel junctions under an electric field.[18] The formulas used to calculate tunneling current density for $\sigma(=\uparrow,\downarrow)$ electrons are[19]

$$J_\sigma(\theta) = \frac{em}{4\pi^2\hbar^3}\int_{-\lambda h_{\rm FM}}^{E_{\rm F}} (E_{\rm F}-E)T_\sigma(\theta)dE, \ eV > E_{\rm F}, \tag{3}$$

$$J_\sigma(\theta) = \frac{em}{4\pi^2\hbar^3}\Big[\int_{-\lambda h_{\rm FM}}^{E_{\rm F}} (E_{\rm F}-E)T_\sigma(\theta)dE + \int_{E_{\rm F}-eV}^{E_{\rm F}} (E_{\rm F}-E)T_\sigma(\theta)dE\Big], \ eV < E_{\rm F}, \tag{4}$$

where $\lambda = \pm$ for $\sigma(=\uparrow,\downarrow)$ electrons, respectively, $T_\sigma(\theta)$ denotes the transmission coefficient of $\sigma(=\uparrow,\downarrow)$ electrons when the angle subtended by magnetization in ferromagnetic electrode and spin-filter barrier is θ, and $E_{\rm F}$ is the Fermi energy of the nonmagnetic electrode.

The spin-polarization of the transport-current can be defined as[17]

$$P = \frac{J_\uparrow(\theta) - J_\downarrow(\theta)}{J_\uparrow(\theta) + J_\downarrow(\theta)}. \tag{5}$$

According to Eqs. (3)–(5), in the following the spin-polarization in the FM/I/SF/NM hybrid tunnel barrier junction on the thicknesses of the barrier, the barrier heights and the molecular fields in the SF layer are investigated. In the calculation, the electron Fermi energy $E_{\rm F}$ in ferromagnetic electrodes is taken as 2.6 eV, $h_{\rm FM}$ is taken as 1.9 eV, and the effective mass of a tunneling electron is taken as the mass of a free electron.[17]

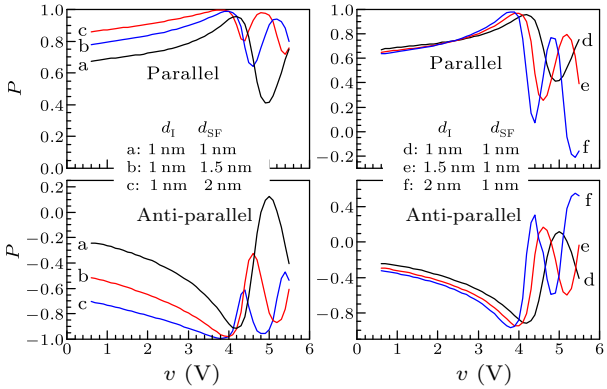

Fig. 2. The variations of P with bias for different barrier thicknesses in parallel and anti-parallel configurations. One case is that the thickness of the I layer is fixed and the thickness of the SF layer is varied. The other case is that the fixed layer and the varying layer are exchanged.

Firstly, the variations of P with bias for different barrier thicknesses are calculated. In the calculation, we assume that the potential barrier heights for two insulator barriers $U_{\rm I}$ and $U_{\rm F}$ are the same, and $U_{\rm I} = U_{\rm F} = 3.0$ eV. In our calculation, the potential barrier heights are all calculated from the Fermi energy. The molecular field in the SF layer is taken as $h_{\rm F} = 0.18$ eV. We maintain the thickness of the I layer $d_{\rm I}$ constant and vary the thickness of the SF layer $d_{\rm F}$ and then vice visa. The results for parallel and antiparallel configuration are shown in Fig. 2. From Fig. 2, we can see that, at the parallel configuration, P is always positive, and at antiparallel configuration, P is always negative. When the bias is smaller than the barrier height, P is almost increasing linear with bias and about $\pm 100\%$ spin-polarization can be obtained in parallel or antiparallel configurations. However, when the bias exceeds the barrier height, the spin-polarization P begins to decrease and if we increase the bias further, the oscillation of P with bias appears. These results indicate that the spin-up (spin-down) electrons cross barriers much more easily than spin-down (spin-up) electrons for the parallel (antiparallel) configuration. In the parallel configuration, when the bias is lower than the barrier height, the electronic tunneling current for spin-up electrons is much larger than that of the spin-down electrons as the spin-up electrons cross a lower barrier height than spin-down electrons, thus P is increasing with the bias firstly. With further increasing the bias voltage, this scene continues and even strengthens with the onset of the Fowler–Nordheim tunneling in spin-up channel (see Fig. 2).[20] However, when the bias is increa-

sed further to exceed the barrier height, the Fowler–Nordheim tunneling is established in the spin-down electrons tunneling as well, P begins decreasing and a turnover point happens. With the strong increase of the tunnel conductance in the spin-down channel, the spin polarization reduces in magnitude and eventually oscillations appear at very high bias. The curves for the antiparallel configuration can be explained in the same way as the parallel configuration just to exchange the behaviors of the spin-up electrons with the spin-down electrons. In addition, from Fig. 2, we can see that the influence of variations of the thickness of the barrier layers on the tendency of the P curve is small, but for the thicker barrier layers, the bias corresponding to the turnover point in the P curve is much smaller, thus the approximate linear variation range of P with the bias is decreased for the thick barrier.

Figure 3 shows the variations of P with bias for different barrier heights. In the calculation, we assume that the potential barrier heights for two insulator barriers $U_{\rm I}$ and $U_{\rm F}$ are the same, $U_{\rm I} = U_{\rm F}$. From Fig. 3, we can see that the position of P peaks shifts systematically toward higher voltages for higher barrier heights. The calculation reveals that the higher barrier heights lead to the larger linear variation regions of P with bias, and thus the higher barrier height is useful for the spin-dependent devices when they need to work at high bias. The reason for the above results can be explained as follows: the linear variation regions of P with bias are related to the occurrence of Fowler–Nordheim tunneling, when the barrier height is increased, the bias for the Fowler–Nordheim tunneling occurrence is also increased, and that leads to the larger linear variation regions of P with bias.

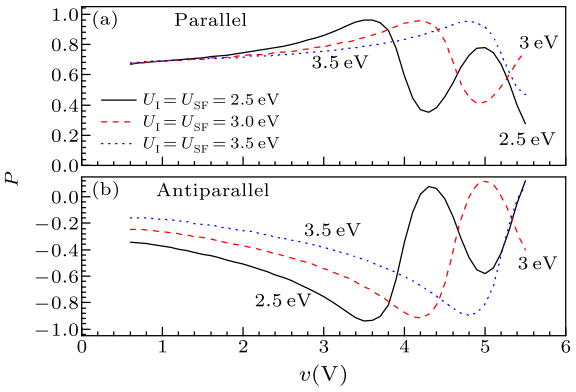

Fig. 3. The variations of P with bias for different barrier heights.

Figure 4 shows the variation of P with the differences of the barrier heights for $U_{\rm I}$ and $U_{\rm F}$. In the calculation, we fix $U_{\rm I} = 3.0$ eV and vary $U_{\rm F}$. The differences of the barrier heights for $U_{\rm I}$ and $U_{\rm F}$ are denoted by $\delta = U_{\rm I} - U_{\rm F}$. From Fig. 4, we can see that the linear variation regions of P with bias increase along with the increase of the $U_{\rm F}$ barrier height. Thus the larger barrier height of $U_{\rm F}$ is favorable when the linearly tuning of P is needed at high bias.

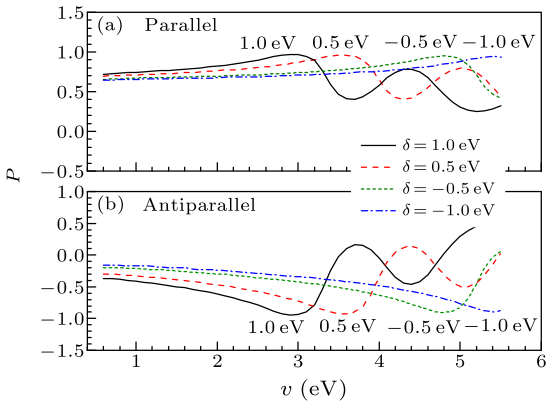

Fig. 4. The variations of P with bias for the differences of the barrier heights δ. The value of $U_{\rm I} = 3.0$ eV is fixed and the difference of the barrier heights for $U_{\rm I}$ and $U_{\rm F}$ is denoted by $\delta = U_{\rm F} - U_{\rm I}$. The thicknesses of I and SF layers are taken to be equal and $d_{\rm I} = d_{\rm F} = 1$ nm. The molecular fields in the FM and SF layers are taken as $h_{\rm FM} = 1.9$ eV and $h_{\rm F} = 0.18$ eV, respectively.

Figure 5 shows the variation of P with bias for different molecular fields in the SF layer. From Fig. 5, we can see that the variations of P with the bias for different molecular fields are almost the same. At the same bias, the larger the molecular field is, the larger the P is. In addition, the turnover points in the curves are the same. These results show that the influence of the molecular field on the Fowler–Nordheim tunneling in the FM/I/SF/NM junction is small.

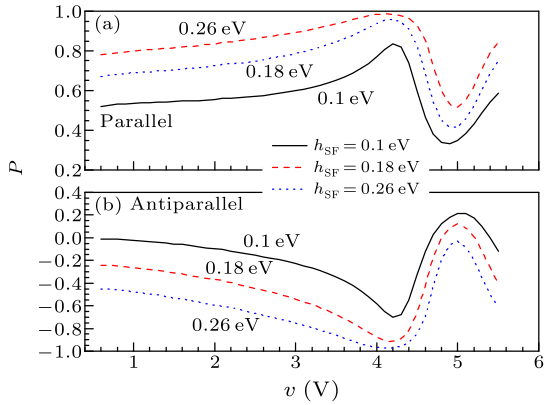

Fig. 5. The variations of P with bias for the different molecular fields in the SF layer. The potential barrier heights for two insulator barriers $U_{\rm I}$ and $U_{\rm F}$ are the same and $U_{\rm I} = U_{\rm F} = 3.0$ eV. The thicknesses of I and SF layers are taken to be equal and $d_{\rm I} = d_{\rm F} = 1$ nm. The molecular field in the FM is taken as $h_{\rm FM} = 1.9$ eV.

In summary, we have calculated the dependence of P on bias in the coherent tunneling regime in FM/I/SF/NM quasi-magnetic tunnel junctions. From the calculations, we can see that at the parallel or antiparallel magnetic configuration, the large positive or negative spin-polarization can be obtained from the FM/I/SF/NM quasi-magnetic tunnel junctions and in a large bias region, the spin-polarizations in FM/I/SF/NM quasi-magnetic tunnel junctions can be linearly adjusted by the bias. The linear variation regions of spin-polarization with bias can be de-

cided by the Fowler–Nordheim tunneling and influenced by the thicknesses and heights of the I and SF barrier layers. The linear variation regions increase with the thickness of the SF barrier layer but decrease with increasing the thickness of the I layer. However, the large barrier thickness can make the large high junction's impedance and low TMR, thus the suitable barrier thickness needs to be carefully selected. The large barrier heights of I and SF layers are beneficial for increasing the linear variation regions especially the barrier height of the SF layer. The variations of molecular field in the SF layer have influence on the value of the spin-polarization but have slight influence on the linear variation regions of spin-polarization with bias. In the calculations, we have not considered the effects of temperature, but have given that the present experiments are most at low temperatures, and we think that our corresponding results may also provide some useful messages in controlling the spin polarizations of a tunnel current in MTJs.

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