Negative tunnelling magnetoresistance in spin filtering magnetic junctions with spin–orbit coupling*

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We present theoretical calculations of spin transport in spin filtering magnetic tunnelling junctions based on the Landauer–Büttiker formalism and taking into account the spin–orbit coupling (SOC). It is shown that spin-flip scattering induced by SOC is stronger in parallel alignment of magnetization of the ferromegnet barrier (FB) and the ferromagnetic electrode than that in antiparallel case. The increase of negative tunnelling magnetoresistance with bias is in agreement with recent experimental observation.

Keywords: tunnelling magnetoresistance, spin filtering barrier, magnetic tunnelling junctions, spin–orbit coupling

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1. Introduction

Spin-polarized transport in nanostructures has been intensively studied since the observation of large tunnelling magnetoresistance (TMR) in magnetic tunnelling junctions (MTJs) at room temperature.[1−5] MTJs consist of two ferromagnetic (FM) leads separated by a thin insulator (I) or semiconductor barrier. A reversal of the relative orientation of the magnetic moments of the two FM layers from antiparallel (AP) to parallel (P) induces a difference in tunnelling resistance between AP and P configurations of the FM layers. This is known as TMR effect, which is quantitatively defined as TMR $= (G_{\rm p} - G_{\rm ap})/G_{\rm ap}$, where $G_{\rm p}$ ($G_{\rm ap}$) is the spin-conserving tunnelling conductance when the magnetic moments of the two FM electrodes are parallel (antiparallel).

The origin of this phenomenon is the spin-dependent band structure (density of states (DOS)) of the FM lead at the Fermi level due to exchange splitting between spin-up and spin-down subbands.[1] In most cases, $G_{\rm p} > G_{\rm ap}$, which means that the TMR is positive. However, the opposite case, i.e., negative TMR is also possible[6] if the transport of carriers is spin or energy dependent.[5] Spin polarization of a given FM electrode has been thought to be a consequence of the intrinsic spin-dependent DOS. Recent findings reveal that the magnitude of the spin polarization and even its sign, can be altered for different barrier materials.[6] Effective polarization of Co has been found to be positive (higher tunnelling probability for majority spin electrons) when Al_2O_3 is used as the insulating barrier and it becomes negative (higher tunnelling probability for minority spin electrons) when $SrTiO_3$ or $Ce_{0.69}La_{0.31}O_{1.845}$ is used as the insulating barrier. Furthermore, the bias dependence of TMR is different between these two cases. The strong influence of the electronic structure of the barrier and barrier–electrode interface on the electron spins raises interesting fundamental questions and presents new ways to tailor the TMR.

To obtain efficient injection of highly spin-polarized electrons, which is essential to the operation of spin electronic devices, much attention has been focused on the development of the structures and the materials involved, mostly FM electrode or FM semiconductor is used as the source for spin polarized carriers.[6,10,11] The alternative to generate spin-polarized current is to use the spin filtering effect, which was first observed when electrons tunnelling through insulating barriers made of Eu chalcogenides.[11−14] With a higher Curie temperature

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and a greater exchange splitting of conduction band, ferromagnetic semiconductor EuO holds promise to reach 100% spin filtering at higher temperatures.[15] Large TMR has been predicted and observed in double spin filtering tunnelling junctions.[16,17] The exponential dependence of tunnelling current on barrier height implies a very efficient spin filtering effect due to the different barrier heights for spin-up and spin-down electrons due to the spin splitting of the energy bands of the FB. Spin injection into semiconductors via tunnelling seems to be the most promising among various possible methods since this process is not affected by the conductivity mismatch at the interfaces.[18] To demonstrate spin filtering by an FB, the spin polarized state of the current after tunnelling through a nonmagnetic electrode can be analysed by a ferromagnetic countre–electrode, which collects the current in different manners depending on whether the spins are parallel or antiparallel to its magnetization.[11]

2. Theoretical treatment

Conduction electrons lose memory of their spin orientation due to spin–orbit coupling (SOC), which stems from the quadratic term in v/c expansion of the Dirac equation,[19]

$$H_{\rm so} = \frac{\hbar}{4m^2c^2}\left(\boldsymbol{\nabla} V \times \boldsymbol{p}\right)\cdot\boldsymbol{\sigma}, \tag{1}$$

where $\boldsymbol{\sigma}$ is Pauli operator, V is the background potential and m is the effective electron mass. SOC provides a spin-dependent potential, which is responsible for spin-flip electron scattering and mixing of spin channels. Effects of SOC on the electron transport properties in the two-dimensional mesoscopic systems have been studied since the early 1980s and attention has been turned to the effects caused by the Rashba term in the case of two-dimensional and quasi-one-dimensional systems, which originates from the structural inversion asymmetry.[3] Recently, the influence of SOC on spin-dependent transport in MTJs was reported[20,21] and a spin-valve-like TMR resulting from strong SOC was observed in the system composed of a single magnetic layer.[22]

Using the spin resolved formalism based on Landauer–Büttiker theory,[20] we investigate the effect of spin filtering and spin-flip scattering on zero-temperature coherent transport properties of spin filtering tunnelling junctions, taking into account SOC induced by scattering potential at the interface within the framework of three dimensional tight-banding model. The technique combines a real space Green function calculation for the leads, implemented with a recursive algorithm for the scattering region (referred to as a sample),[25] details of the method can be found in Ref. [20]. Our numerical treatment is spin-resolved, thus enabling us to identify quantitatively the contributions to the transport property by different spin channels and the ratio of spin-flip conductance due to spin–orbit scattering at the interface—issues which are intrinsic and thus are vital to our understanding of spin transport phenomena. Our results predict a negative TMR ratio, i.e., tunnelling conductance is larger when the relative magnetization of the FB and the FM electrode is antiparallel than that when it is parallel for both NM/FB/FM (type I) and NM/FB/FM/NM (type II) junctions considered. In particular, we find that the bias dependence of TMR is quite different in these two cases due to the presence of right NM electrode. Our calculations reveal that negative TMR is an intrinsic property of some spin filtering tunnelling junctions, which occurs due to the combined effect of a spin filtering barrier and an FM electrode. Though tunnelling conductance is suppressed by SOC, spin polarization or TMR may be enhanced or suppressed depending on the tunnelling structures.

Since s bands should be able to couple most efficiently across the interface and decay most slowly in the barrier as suggested in recent studies,[24] the electronic structure of the whole system is described by an orthonormal nearest-neighbour single-orbit tight-binding model with hopping integral t, spin-dependent conductance is calculated in terms of spin-dependent total transmission coefficient[20] at Fermi energy.

Taking into account spin-flip scattering induced by SOC, the spin-resolved conductance is the sum of the spin-conserving and the spin-flip components due to the mixing of spin channels induced by SOC,

$$G = G_{\rm sc} + G_{\rm sf}, \tag{2a}$$

$$G_{\rm sc} = G_{\rm uu} + G_{\rm dd}, \tag{2b}$$

$$G_{\rm sf} = G_{\rm ud} + G_{\rm du}, \tag{2c}$$

where $G_{\rm sc}$ and $G_{\rm sf}$ are spin-conserving and spin-flip components of conductance, respectively, u(d) represents up spin (minority spin) (down spin (majority spin)) whose magnetic moments are antiparallel (parallel) to the magnetization of the FB and the FM, respectively. To evaluate the influence of spin-flip scattering on the tunnelling process due to SOC, we define

the ratio of the spin-flip conductance by

$$G_{\rm sfr} = \frac{G_{\rm sf}}{G}. \tag{3}$$

TMR is written as

$$\mathrm{TMR} = 2 \times \frac{G_{\rm p} - G_{\rm ap}}{G_{\rm p} + G_{\rm ap}}, \tag{4}$$

where $G_{\rm p}$ ($G_{\rm ap}$) is the total tunnelling conductance (TC) when the magnetizations of the FB and the FM are parallel (antiparallel).

3. Results and discussion

Using the above technique, we performed numerical calculations for Cu/EuO/Co and Cu/EuO/Co/Cu hybrid spin filtering tunnelling junctions,[25] which have a similar structure to those devices proposed.[11,12,26] The magnetization orientation of the spin filtering barrier and the FM electrode can be changed independently,[11] thus both parallel and nearly antiparallel alignments can be achieved. The tight-binding parameters employed in our calculations are obtained from the band structures of fcc Co, Cu and from known experimental values of exchange splitting and on-site energy for ferromagnetic semiconductor EuO.[16,27,28] Spin–orbit coupling parameter is chosen based on the analysis of spin relaxation length due to SOC.[29] In our calculations, ferromagnetic barrier and ferromagnetic layer in NM/FB/FM/NM structure is fixed at four and three atomic layers, respectively; otherwise, the right FM electrode in NM/FB/FM junction is semi-infinite. We consider a unit cell containing up to 10×10 atoms and impose periodic boundary conditions in the plane perpendicular to the current direction

Spin-resolved conductance (Figs. 1(a), 1(b), 2(a) and 2(b)) and total conductance (Figs. 1(c) and 2(c)) are shown as a function of bias voltage in Cu/EuO/Co and Cu/EuO/Co/Cu tunnelling junctions with and without spin–orbit coupling, respectively. As seen from Figs. 1(a), 1(b), 2(a) and 2(b), minority spin (uu_p) electron dominates tunnelling process in parallel configuration for both structures and the conductance is a linear function of bias with positive slope for Cu/EuO/Co structure; otherwise, it follows a parabolic relation with respect to bias for Cu/EuO/Co/Cu structure, while the majority spin conductance (dd_p) shows a linear variation, with a small negative slope, with bias in parallel configuration of both Cu/EuO/Co and Cu/EuO/Co/Cu structures. Significant difference between the conductance by minority and majority spins appears in antiparallel configuration (see du_p and ud_p). Except for du_ap, the conductance shows small variations with bias in antiparallel configuration for both junctions.

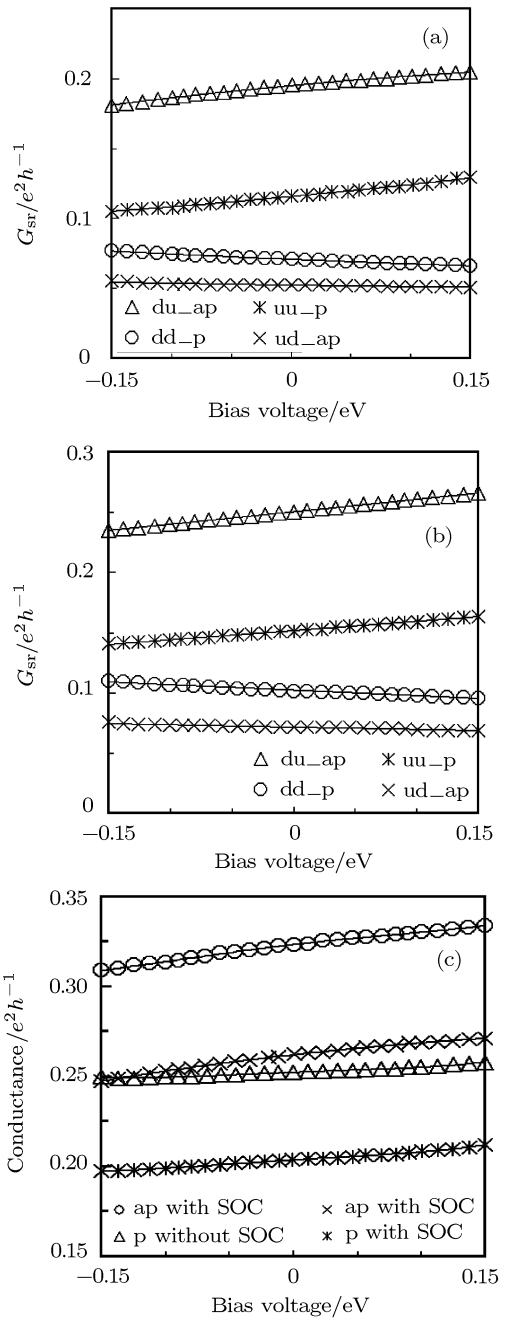


Fig. 1. Spin-resolved and total tunnelling conductance versus bias voltage in parallel and antiparallel configurations for Cu/EuO/Co tunnelling junctions, respectively (spin-resolved conductance: (a) without spin–orbit coupling, (b) with spin–orbit coupling; (c) total tunnelling conductance). See the text for the definitions of u and d.

The above behaviour arises due to the combined effect of spin filtering and band structures (DOS) of Co and Cu at the interface between them. For ferromagnetic barrier, the barrier height is spin-dependent,

i.e., majority and minority spins experience different barrier heights due to spin splitting of the conduction band of the FB. Majority electrons have higher tunnelling probability due to the lower barrier height. On the other hand, the DOS of Co at the Fermi level is higher for minority spins.[6]

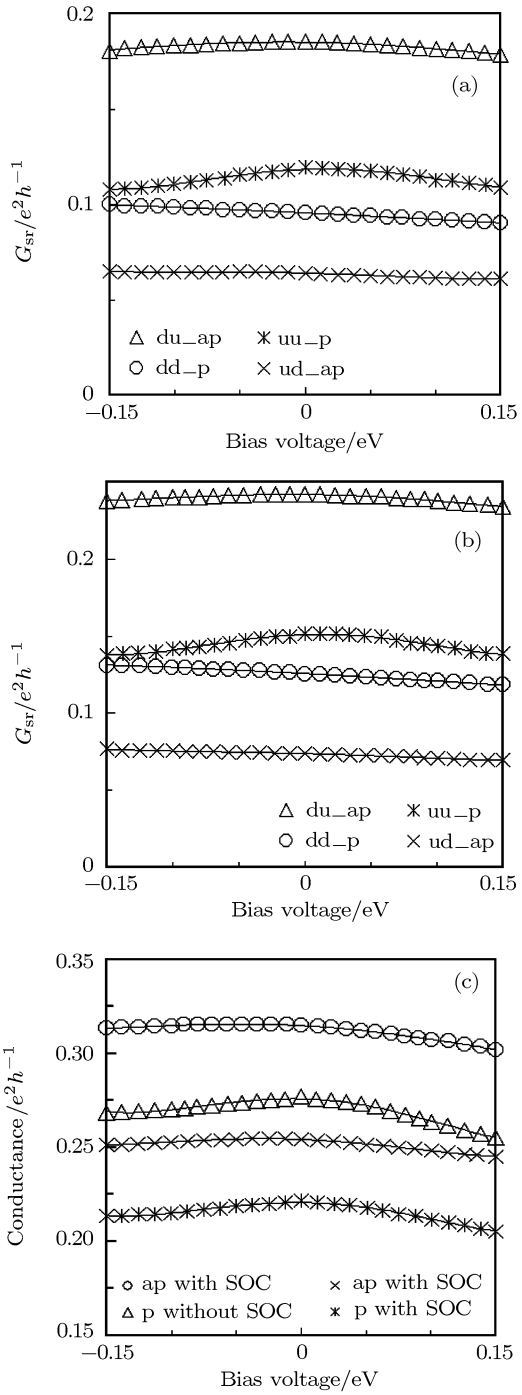


Fig. 2. Spin-resolved and total tunnelling conductance versus bias voltage in parallel and antiparallel configurations for Cu/EuO/Co/Cu tunnelling junctions, respectively, (a), (b) and (c) are similar to that in Fig. 1.

Therefore, dominant contribution to the tunnelling conductance comes from the majority spin electrons with respect to the ferromagnetic barrier, which enter the minority spin state of the Co layer in antiparallel alignment (i.e., du_ap). Figures 1(a), 1(b), 2(a) and 2(b) confirm our predictions. On the other hand, in the parallel alignment, minority electrons have a slightly higher conductance (see uu_p in Figs. 1(a), 1(b), 2(a) and 2(b)). The decrease of conductance by minority electrons for both positive and negative applied bias in parallel alignment for Cu/EuO/Co/Cu junctions (see uu_p in Figs. 2(a) and 2(b)) reflects the influence of the right Co/Cu interface. As is well known, Cu band is well-matched to the majority sub-band of Co but poorly matched to the minority sub-band.[28] Consequently, majority states suffer little reflection at the Co/Cu interface whereas minority states undergo large inter-band scattering. Thus the combined effect of spin filtering and the band structures (DOS) of the FM electrode induce large tunnelling current in antiparallel alignment as shown in Figs. 1(c) and 2(c). Though characteristic feature of transport does not show sensitive dependence on spin–orbit coupling as shown in Figs. 1(b) and 2(b), the spin-resolved as well as the total conductance shows some suppression due to the SOC in both alignments for both structures. Our results of the tunnelling conductance versus bias are consistent with those obtained by the *ab initio* calculations of bias-dependent conductance of epitaxial systems assuming ideal interfaces.[30]

To evaluate quantitatively the effects of spin-flip scattering on the transport properties, we plot the ratio of spin-flip conductance versus bias in Fig. 3, which shows a distinct dependence intrinsic to the structure and the relative orientation of magnetization of the FB and the FM. Our calculations indicate stronger spin-flip scattering in parallel alignment than in antiparallel alignment for both structures. In addition, though the spin-flip scattering is more pronounced for Cu/EuO/Co junctions than for Cu/EuO/Co/Cu in parallel alignment for negative bias, they show only small variations in this region; however, opposite tendency is predicted for positive bias, which reflects the influence of scattering at the Co/Cu interface. On the other hand, the spin-flip scattering decreases gradually with negative bias for Cu/EuO/Co junctions when the magnetic moments of FB and FM are antiparallel to each other and tends to be indistinguishable with that for Cu/EuO/Co/Cu structures as positive bias increases.

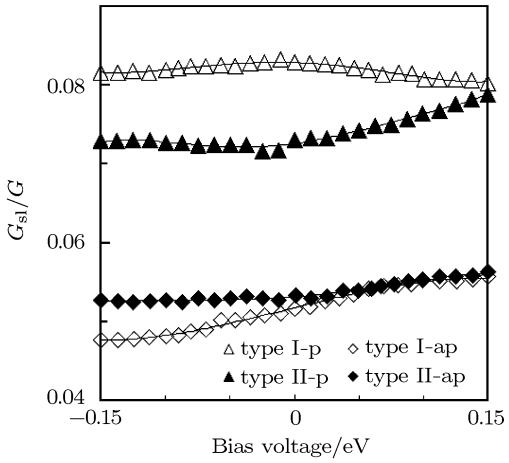


Fig. 3. The ratio of spin-flip conductance versus bias voltage for Cu/EuO/Co (empty triangle: parallel alignment; empty square: antiparallel alignment) and Cu/EuO/Co/Cu (filled triangle: parallel alignment; filled square: antiparallel alignment) tunnelling junctions, respectively.

Such a behaviour can be understood as follows. As demonstrated in Figs. 1(c) and 2(c), tunnelling conductance is larger when the magnetization of the FB and FM are antiparallel to each other, i.e., $G_{\rm ap} > G_{\rm p}$, due to the combined effects of spin filtering and spin-dependent band structure (DOS) of the FM electrode. As explained above, this gives a negative TMR effect as shown in Fig. 4. However, spin-flip conductance is expected to be larger in parallel configuration than in antiparallel. The reason is the reversal of the DOS of up-spin and down-spin electrons for electrons which undergo spin-flip scattering. In other words, from the viewpoint of the tunnelling electrons which change their spin orientation during tunnelling process, it seems as if the magnetization of the right ferromagnetic electrode was reverted.

Figure 4 shows bias dependence of TMR, which is quite different for the two types of junctions considered. The magnitude of the negative TMR decreases as bias increases for Cu/EuO/Co structures, while it increases for Cu/EuO/Co/Cu junctions due to the obviously different bias dependence of the total tunnelling conductance. However, the total conductance shows a substantial decrease with both positive and negative biases for Cu/EuO/Co/Cu junction in parallel alignment. As a result, the difference between $G_{\rm p}$ and $G_{\rm ap}$ increases with both positive and negative biases, leading to the stronger dependence of the absolute magnitudes of TMR ratio on bias as shown in Fig. 4 (filled and empty circles). In general, TMR decreases with bias, which can be a detrimental factor to practical applications, since most devices require a relatively bias-independent magnetoresistance to allow stable operation. In our simulation, the increase of TMR ratio with bias (see Fig. 4) is in agreement with recent experimental observations.[12] We note that spin–orbit coupling enhances the negative TMR except for positive bias in Cu/EuO/Co junctions due to the different bias dependence of the total tunnelling conductance in parallel and antiparallel alignments, respectively (see Figs. 1(c) and 2(c)).

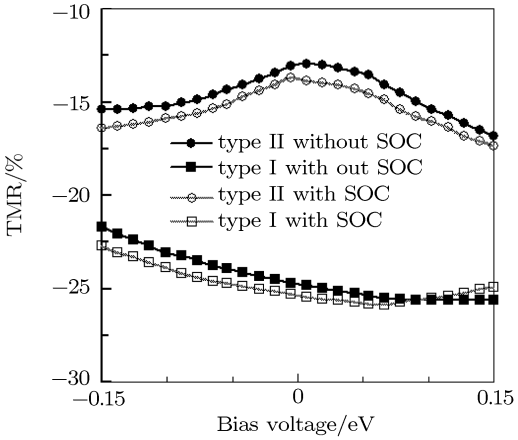


Fig. 4. TMR versus bias voltage for Cu/EuO/Co/Cu (filled circle: without spin–orbit coupling; empty circle: with spin–orbit coupling) and Cu/EuO/Co (filled square: without spin–orbit coupling; empty square: with spin–orbit coupling) tunnelling junctions, respectively.

4. Conclusion

We have investigated spin-dependent electron transport of spin filtering magnetic tunneling junctions taking into account spin–orbit coupling. The conductivity is suppressed by SOC, while TMR is either enhanced or suppressed depending on the structures considered. We show the feasibility to modulate the TMR through the design of the junction structures and to control the spin polarisation with potential application in spintronic devices in negative magnetoresistance regime, which has potential utility as spin injection devices into semiconductors.

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