Spin Transport in Spin Filtering Magnetic Tunneling Junctions

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Taking into account spin-orbit coupling and s–d interaction, we investigate spin transport properties of the magnetic tunneling junctions with spin filtering barrier using Landauer-Büttiker formalism implemented with the recursive algorithm to calculate the real-space Green function. We predict completely different bias dependence of negative tunnel magnetoresistance (TMR) between the systems composed of nonmagnetic electrode (NM)/ferromagnetic barrier (FB)/ferromagnet (FM) and NM/FB/FM/NM spin filtering tunnel junctions (SFTJs). Analyses of the results provide us possible ways of designing the systems which modulate the TMR in the negative magnetoresistance regime.

Keywords: Magnetic Tunneling Junctions, Spin Polarized Transport, Spin Filtering, Spin-Orbit Coupling, Tunneling Magneto-Resistance.

1. INTRODUCTION

Spin-polarized transport in nanostructure has recently attracted a great deal of attention and been extensively studied after the observation of large room temperature tunneling magneto-resistance (TMR) through magnetic tunneling junction (MTJ)\textsuperscript{1,2} which consists of two ferromagnet (FM) leads separated by a thin insulator (I) or semiconductor barrier. A reversal of orientation of the magnetization of the two FMs from anti-parallel (AP) to parallel (P) by applying a magnetic field produces so called TMR effect. The magnitude of the TMR effect is defined as the difference between the tunnel resistance of AP configuration and that of P configuration of the magnetization, which can be formulated as $TMR = (G_p - G_{ap})/G_{ap}$, where $G_p$ ($G_{ap}$) is the spin-conserving tunnel conductance when the magnetizations of the two FM electrodes are aligned parallel (antiparallel), respectively. In most cases, $G_p \gg G_{ap}$, which causes TMR to be positive. However, the opposite case can occur. TMR becomes negative\textsuperscript{3} if the transport of carriers is spin or energy dependent.\textsuperscript{4} Spin polarization of electrons tunneling from a given FM electrode was generally thought that it reflects the intrinsic spin polarization of density of state (DOS) of the FM electrode. Recent findings show that the magnitude of spin polarization, and even its sign, depends on the choice of the barrier material.\textsuperscript{5}

Efficient injection of highly spin-polarized electrons is essential for the operation of spin electronic devices. Many studies employ a FM electrode or a FM semiconductor as a source of spin polarized carrier.\textsuperscript{5–4} Another way to generate the current of highly spin polarized electrons is to use spin filtering effect, which has been observed previously when electrons tunnel through insulating barriers made of Eu chalcogenides or BiMnO\textsubscript{3} and EuO.\textsuperscript{10–13} To demonstrate spin filtering by a ferromagnetic barrier, the spin polarization of the current can be analyzed with a ferromagnetic counter-electrode (CE).\textsuperscript{14} Then the resulting current should be dependent on the relative orientation between the magnetic moments of the ferromagnetic barrier and the CE. There is still a need for fundamental study before the potential of applications be fully realized.

2. THEORETICAL MODEL

Conduction electrons lose memory of their spin orientation due to spin-orbit coupling (SOC) which stems directly from the quadratic term in $r/c$ expansion of the Dirac equation.\textsuperscript{15} Taking into account the SO coupling and local s–d exchange interaction, the second quantization expression for Hamiltonian is given by\textsuperscript{16}

\begin{equation}
H = \sum_{r, \alpha, \beta} \left( v_{r} \delta_{\alpha \beta} + \frac{\gamma_{r}}{2} \mu_{\alpha} \cdot \sigma_{\alpha \beta} \right) c_{r, \alpha}^{+} c_{r, \beta} + t \sum_{(r, r') \alpha} c_{r', \alpha}^{+} c_{r, \alpha} + \sum_{r, \alpha} \Phi_{r} c_{r, \alpha}^{+} c_{r, \alpha} + H_{sc} \quad (1a)
\end{equation}

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$H_{so} = i \xi_{so} \sum_{r, \alpha, \beta} \left[ \Delta e_{r+i, \alpha, \beta} c_{r+i, \alpha, \beta}^+ c_{r, \alpha, \beta} \sigma_{\alpha \beta}^z + \Delta e_{r+i, \alpha, \beta} c_{r+i, \alpha, \beta}^+ c_{r, \alpha, \beta \sigma_{\alpha \beta}} + \Delta e_{r+i, \alpha, \beta}^+ c_{r+i, \alpha, \beta}^+ c_{r, \alpha, \beta \sigma_{\alpha \beta}} \right] (1b)$

$$t = - \frac{\hbar^2}{2m^* a^2} (1c)$$

where $r$ and $\alpha (\beta)$ are spatial and spin indices, respectively, $\gamma_r$ the exchange splitting at magnetic site, $\delta_{\alpha \beta}$ the delta function, $\vec{\mu}$, the unit vector in the direction of magnetization, and $m^*$ and $h$ the effective mass of electron and Planck constant, respectively. $\xi_{so}$ spin-orbit parameter, $(\sigma_{\alpha \beta})$ the Pauli operator with $\sigma_{\alpha \beta}$, and $\sigma_{\alpha \beta}$ matrix elements of the Pauli operator, $\Phi_r$ the electrostatic potential with $\Phi_r = eV$ on the left electrode and $0$ on the right electrode, which is valid for small bias voltage $V$. We follow standard notations of the second quantization formalism, so $c_{r, \alpha}^+$ ($c_{r, \alpha}$) denotes the creation (annihilation) operator with spin $\alpha$ at site $r$, $e_r$ the on-site energy, $r = a \pm a$, the nearest-neighbor sites from site $r$ along $y$ (z) axis, $a$, ($a$) the vector paralling to the $y$ ($z$) axis with the lattice constant $a$, and finally $\Delta e_{r+i, \alpha, \beta} = e_{r+i, \alpha, \beta} - e_{r, \alpha, \beta}$. The summation over nearest-neighbor hopping sites. All energies are measured in unit of nearest-neighbor hopping integral $|t|$, which is same for all pairs of nearest neighbors.

The general setup of the system is two semi-infinite ideal electrodes separated by a sample (scattering region), which is same simple cubic lattice structure and an array of atomic layers along [100] (current) direction (namely, the $x$ axis) with lattice parameter $a$. A periodic structure of $N_x \times N_y$ supercell is considered, where $N_x$ and $N_y$ are numbers of the sites along the $x$ and $y$ axes, respectively. Since it is transparent physically, the electronic structure of the whole system is described by an orthonormal nearest-neighbor single-orbit tight-binding model with hopping integral $t$. The s-d exchange splitting induces relative shift between majority and minority spin subbands of FB and FM. Coherent transport properties were studied using the Landauer-Büttiker theory, and the spin-dependent conductance was obtained in terms of the spin-dependent total transmission coefficient at the Fermi energy. We define TMR ratio as

$$\text{TMR} = 2 \times \frac{G_p - G_{ap}}{G_p + G_{ap}} (2)$$

where $G_p (G_{ap})$ is the total tunneling conductance (TC) when the orientations of the magnetization of FB and FM is aligned parallel (anti-parallel) each other.

### 3. RESULTS AND DISCUSSION

We studied spin transport properties of hybrid spin filtering tunneling devices made of NM|FB|FM, in analogy with the half-metallic ferromagnet|insulator|ferromagnet tunneling junctions, without and with the right NM lead, respectively. In the present calculations, the thickness of barrier and ferromagnetic layer in NM|FB|FM structure is fixed at three and four atomic layers, respectively. Otherwise a semi-infinite electrode is used for the right ferromagnetic electrode in NM|FB|FM junction. The tight-binding parameters employed in our calculations were chosen so that they can be well fitted to the calculated results of accurate first-principle calculation of the band structures of fcc Co, Cu, and the known experimental values of exchange splitting, and on-site energy of the ferromagnetic semiconductor EuO. Spin-orbit coupling parameter was chosen as 0.1 from the analysis of the spin relaxation length induced by the SOC. Total tunneling conductance is calculated as we increase $N_x$ and $N_y$ up to 10 and confirmed that the change of the total tunneling conductance is negligible at this level.

Figure 1 shows total conductance (Figs. 1(a) and (b)) as a function of applied bias voltage for Cu/EuO/Co (type I) junction and Cu/EuO/Co/Cu (type II) junction with and without spin-orbit coupling, respectively. The spin filtering effect and band structures (DOS) at the interfaces give the parallel and antiparallel conductance, with each having a unique dependence on the bias voltage. Obviously qualitative feature of the transport does not depend on the presence of spin-orbit coupling, even though it shows some quantitative change depending on the structure. As can be seen in Figures 1(a) and (b), the total conductance is suppressed by the SOC for all cases. Tunnel conductance is relatively larger when the relative orientation of magnetization between the FB and FM is antiparallel to each other, i.e., $G_{ap} > G_p$, due to the combined spin filtering and spin dependent DOS at the interface. This gives a negative TMR effect as shown in Figure 2.

Figure 2 shows TMR versus bias voltage curve which demonstrates structure dependent transport characteristics. The figure clearly shows that the magnitude of the negative TMR decreases with increase of bias voltage in type I junctions, whereas it increases in the type II junctions. As shown in Figures 1(a) and (b), the total TC has linear relation with bias voltage in type I junctions with a slightly larger slope in the antiparallel alignment. Hence, the difference between $G_p$ and $G_{ap}$ increase with increasing the bias voltage, which resulting in the shifted parabolic bias.

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**Fig. 1.** Total tunnel conductance as a function of applied bias in type I (a) and type II (b) tunneling structures with and without spin-orbit coupling for parallel and antiparallel configurations, respectively.

dependence of TMR due to the asymmetric structure as shown in Figure 2 (solid and dot-dashed lines). However, the total tunnel conductance decreases for both positive and negative bias voltages in type II junctions distinctly in the parallel alignment, thus the difference between $G_p$ and $G_{np}$ increase for both positive and negative bias voltages, which leads to the increasing dependence of the absolute magnitudes of TMR ratio on the bias voltage (see Fig. 2, dashed and dotted lines). A critical aspect of magnetic junctions is the bias dependence of TMR, which, in general, decreases as the bias voltage increases, and is detrimental for practical applications since most practical applications require a relatively bias-independent magnetoresistance to have stable device operations. In the present calculations, the variation of TMR ratio with bias is very slow (see Fig. 2) as compared with those reported so far. We note that spin-orbit coupling has a profound effect on TMR ratio in type II structure due to the presence of the Co/Cu interface, and the absolute magnitude of negative TMR is enhanced; on the contrary, it decreases in type I structures, and a crossover occurs between the two TMR versus bias curves beyond a certain positive voltage due to the different slope of bias dependence of the total tunnel conductance in parallel and anti-parallel alignments (see Figs. 1(a) and (b)).

4. CONCLUSION

We investigated the spin polarized transport properties of the tunneling junctions consisting of spin filtering barrier and a ferromagnetic electrode taking into account both spin-orbit coupling and s–d interaction, and predicted completely different bias voltage dependence of negative TMR for Cu/EuO/Cu and Cu/EuO/Co/Cu structures, which originates from the combined effects of spin filtering and band structures at the interfaces. Though tunnel conductance is suppressed by SOC, the spin polarization or TMR may be enhanced or depressed depend on the tunnel structures considered. We demonstrated theoretically the feasibility to modulate the TMR by design of system structure, and presented the way to control the spin polarization useful for potential application of the spintronic devices in negative magnetoresistance regime.

Acknowledgments: The work was initiated at National Creative Research Initiative Center for Superfunctional Materials, Pohang University of Science and Technology, South Korea, and is supported in part by the NSFC Grant No. 10564004, the Natural Science Foundation of Yunnan Province Grant No. 2004C0007M, and Korea Research Foundation Grant No. KRF-2005-070-C00065.

References and Notes


Received: 13 April 2007. Revised/Accepted: 31 May 2007.