A two-band model of spin-polarized transport in Fe/Cr/MgO/Fe magnetic tunnel junctions

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Theoretical studies of spin dependent transport in Fe/Cr/MgO/Fe tunnel junctions with noncollinear alignment of magnetizations of metallic layers comprising these magnetic tunnel junctions are presented. Calculations are performed with use of nonequilibrium Green function technique in the framework of the Keldysh formalism. Electronic band structure of ferromagnetic electrodes is modeled within a two-band model with majority and minority states being *s*-like and *d*-like electrons, respectively. Furthermore, interfacial *s*-*d* hybridization is taken into account and calculated using perturbation corrections for the wave and Green functions. It is shown that in the presence of Cr layer at the Fe/MgO interface, the contribution from *s*-*d* hybridization to the total current is much stronger in the antiparallel magnetizations configuration compared to the parallel one leading to decrease in tunnel magnetoresistance values in agreement with earlier reports.
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I. INTRODUCTION

Magnetic tunnel junctions (MTJs) have been objects of great interest for both scientists and engineers because of their high sensitivity to magnetic fields, which makes them good candidates for hard drive read heads and magnetic random access memories[1,2] (MRAM). The most attractive among MTJs are their crystalline counterparts due to prediction[3,4] and observation[5–7] of large tunnel magnetoresistance (TMR) values due to spin filtering[8] of Bloch states with certain symmetries in Fe/MgO(001) junctions. It was demonstrated using *ab initio* calculations[3,4,8,9] that the "*s*-like" band with Δ_1 symmetry (existing at the Fermi energy only for "up" spins in bcc-Fe (Co and CoFe) along (001) direction) has the smallest decay rate MgO due to evanescent state of the same character in this insulator leading to the high conductance in parallel (P) magnetizations configuration of adjacent ferromagnetic electrodes. At the same time, the conductance in antiparallel (AP) magnetizations configuration yields very small conductance values since there is no *s*-like band for "down" spins in aforementioned bcc ferromagnets but "*d*-like" bands with Δ_2, $\Delta_{2'}$, and Δ_5 symmetries.

Recent exciting experiments[10] demonstrated that additional Cr layer of thickness *a* inserted at the interface between Fe and MgO layers can be used as a tunnel "barrier" for *s*-like electronic states with Δ_1 symmetry providing straightforward evidence of Bloch states symmetry-based spin filtering. In certain sense, bcc-Fe (Co and CoFe) in MgO-based crystalline MTJs should demonstrate "half-metallic"-like behavior leading to huge TMR values. However, in aforementioned experiment[10] with Fe/Cr/MgO/Fe the TMR strongly decreased as a function of Cr thickness and the highest experimental value reported so far in CoFe/MgO/CoFe structures is 600% at room temperature.[11]

One of the possible reasons preventing infinite TMR values can be appearance of the partial layer of FeO at the interface which represents an additional barrier for *s*-electron.[8,12] Another reason could be a symmetry break at the Fe/MgO and/or Cr/MgO interface which in turn leads to the *s*-*d* hybridization with transition to the conducting state in the AP configuration of magnetizations in Fe electrodes. On another hand, Fe/Cr/MgO/Fe structures are likely to have a very similar crystallographic structure as bcc-Fe/Cr/Fe multilayers in which giant magnetoresistance[13] was discovered. Consequently, we do not expect any significant depolarization of conduction electrons in the Cr layer due to its possible antiferromagnetic character.

In this work we theoretically investigate the influence of *s*-*d* hybridization on TMR in Fe/Cr/MgO/Fe and Fe/MgO/Fe structures with noncollinear alignment of magnetizations of ferromagnetic layers comprising these MTJs.

II. MODEL

For sake of simplicity and in a view of arguments stated above, we will describe electronic structure of ferromagnetic electrodes within two bands model, i.e., with majority *s*-like electrons and minority *d*-like holes. It follows from this model that *s*-electron as well as *d*-hole bands have zero conductivity in the case of the AP configuration of magnetizations in the outer ferromagnetic layers, so the TMR in this structure has to reach infinite value. To calculate the conductivity in this noncollinear structure we will use the Keldysh technique for nonequilibrium Green functions[14] with the perturbation corrections coming from *s*-*d* hybridization. Wentzel–Kramers–Brillouin approximation will be used for wave and Green functions in the trapezoidal barrier region under applied voltage.[15] To improve further the model we consider different effective mass for electron and hole bands in each layer. The details of this approach modified for tunnel transport could be found in Ref. 15. To take into account

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s-d hybridization one need to find corresponding corrections to the wave functions using the following matrix equation:

$$\psi^{\sigma}_{s(d)}(z) = \psi^{\sigma}_{0s(d)}(z) + \sum G^{\sigma\sigma'}_{s(d)}(z,z_i)\gamma^{\sigma\sigma'}\psi^{\sigma'}_{d(s)}(z) \tag{1}$$

where $\psi^{\uparrow(\downarrow)}_{0s(d)}(z)$, $\psi^{\uparrow(\downarrow)}_{s(d)}(z)$ are zero order on hybridization and full wave functions for s, d carriers and for up, down spins, $G^{\sigma\sigma'}_{s(d)}(z,z_i)$—retarded Green functions for s, d carriers, z_i—is the metal/barrier interfacial coordinate (the z axis is perpendicular to the interfaces), and $\gamma^{\sigma\sigma}_i$—are the parameters of hybridization on the ith interface. It follows from Eq. (1) that the most important is assumed to be the hybridization at the metal/insulator interface. In general, there are also terms proportional to the off-diagonal on spin parameters of hybridization due to the spin-orbit coupling which is neglected here so it's reasonable to assume that $\gamma^{\sigma,-\sigma}_i \ll \gamma^{\sigma\sigma}_i$. All wave and Green functions depend on energy E of tunneling carriers and on in-plane momentum $\vec{\kappa}$ but for simplicity we will omit these dependences in expressions below. To find the current we have to build the nonequilibrium Green function

$$G^{-+}_{\sigma\sigma\kappa}(z,z') = \mathrm{f}(E)\psi^{\sigma\sigma*}_l(z')\psi^{\sigma\sigma}_l(z) + \mathrm{f}(E-eV)\psi^{\sigma\sigma*}_r(z')\psi^{\sigma\sigma}_r(z), \tag{2}$$

where indexes l, r mean that they are the functions for left-right and right-left moving carriers correspondingly, $\mathrm{f}(E)$, $\mathrm{f}(E-eV)$—are the Fermi distributions in left, right electrodes, and $\vec{\kappa}$ is the momentum along the interface. Then the current is calculated using the formula

$$j^{\sigma} \propto i\int\int \kappa d\kappa dE\left(\frac{\partial}{\partial z'} - \frac{\partial}{\partial z}\right)G^{-+}_{\sigma\sigma\kappa}(z,z')|_{z=z'}. \tag{3}$$

The zero order spin up s-current and spin down d-current are given by the integrals:

$$j^{\uparrow(\downarrow)}_{0s(d)} = C\int\int \kappa d\kappa dE j^{\uparrow(\downarrow)}_{0s(d)}(E,\kappa). \tag{4}$$

As an example, the corresponding integrand for majority spin s-current is defined as:

$$j^{\uparrow(\downarrow)}_{0s(d)}(E,\kappa) = \frac{q_1 q_2 \,\mathrm{Re}\, k_1|k_3|^2 m_1 m_3^2 m_b^2}{|den|^2}[(1+\cos\theta) \times \mathrm{Re}\, k_4 m_1|K(q_2m_2 - ik_5m_b)\varphi^{\downarrow}_2 - K^{-1}(q_2m_2 - ik_5m_b)\varphi^{\downarrow}_4|^2 + (1-\cos\theta)\mathrm{Re}\, k_5 m_2|K(q_2m_1 - ik_4m_b)\varphi^{\downarrow}_2 - K^{-1}(q_2m_1 - ik_4m_b)\varphi^{\downarrow}_4|^2], \tag{5}$$

where

$$K = \exp\int_{z_2}^{z_3} q(z)dz, \quad q^2(z) = \frac{2m_b}{\hbar^2}\left(U - E_e - eV\frac{z-z_2}{z_3-z_2}\right) + \kappa^2,$$

and $q_{1(2)} = q(z_{2(3)})$.

In expressions above z_2, z_3 represent coordinates of the Cr/MgO and MgO/Fe interfaces, respectively; V is the voltage, θ is the angle between magnetizations of Fe layers, $C = 0.1385 m_1^{-1} \times 10^{13}$ A/cm^2, m_1, m_2—are normalized effective mass for s-electron with up, down spin in Fe electrodes, m_3, m_b are the same in Cr and the barrier layers. Furthermore,

$$den = (1+\cos\theta)[K(q_2m_1 - ik_4m_b)\varphi^{\uparrow}_2 - K^{-1}(q_2m_1 + ik_4m_b)\varphi^{\uparrow}_4] \times [K(q_2m_2 - ik_5m_b)\varphi^{\downarrow}_2 - K^{-1}(q_2m_2 + ik_5m_b)\varphi^{\downarrow}_4] + (1-\cos\theta)[K(q_2m_2 - ik_5m_b)\varphi^{\uparrow}_2 - K^{-1}(q_2m_1 + ik_5m_b)\varphi^{\uparrow}_4][K(q_2m_1 - ik_4m_b)\varphi^{\downarrow}_2 - K^{-1}(q_2m_1 + ik_4m_b)\varphi^{\downarrow}_4]$$

$$\varphi^{\uparrow(\downarrow)}_2 = e^{ik_3a}(m_{1(2)}k_3 - k_{1(2)}m_3)(q_1m_3 + ik_3m_b) + e^{-ik_3a}(m_{1(2)}k_3 - k_{1(2)}m_3)(q_1m_3 + ik_3m_b);$$

$$\varphi^{\uparrow(\downarrow)}_4 = e^{ik_3a}(m_{1(2)}k_3 - k_{1(2)}m_3)(q_1m_3 + ik_3m_b) + e^{-ik_3a}(m_{1(2)}k_3 - k_{1(2)}m_3)(q_1m_3 + ik_3m_b);$$

where k_1, k_4 (k_2, k_5) indicate z-components of s-electron momentum with energy E for up, down spins in the left (right) electrodes, and k_3 is the same Cr layer:

$$k^2_{1(2)} = \frac{2m_{1(2)}}{\hbar^2}(E - U_s \pm J_{sd}) - \kappa^2;$$

$$k^2_{4(5)} = \frac{2m_{1(2)}}{\hbar^2}(E - U_s \pm J_{sd} + eV) - \kappa^2;$$

$$k^2_3 = \frac{2m_3}{\hbar^2}(E - U^{\mathrm{Cr}}_s) - \kappa^2.$$

Here U_s—is the bottom of s-band in Fe without exchange splitting J_{sd}, U^{Cr}_s-the same for Cr layer. Similar expressions have been obtained for $J^{\downarrow}_{0d}(E,\kappa)$ with corresponding parameters for d electrons with minority spin (e.g., k^d_2, m^d_1, etc.).

Note that in our model the bottom of electron s-band is situated above the Fermi level giving rise to purely imaginary value for k_3 As it follows from Eqs. (4) and (5) for purely imaginary k_5 (as well as k^d_4 for d electrons, which is the case in our model), and $\theta = \pi$, both s-currents and d-currents vanishes giving TMR$\to\infty$.

In the presence of s-d hybridization additional terms in wave functions appear, for example:

$$\Delta\psi^{\uparrow(\uparrow)}_s(z < z_1) = G^{\uparrow\uparrow}_s(z,z_1)\gamma^{\uparrow\uparrow}_i G^{\uparrow\uparrow}_d(z_i,z_i)\gamma^{\uparrow\uparrow}_i\psi^{\uparrow(\uparrow)}_s(z_i)$$

Taking into account additional terms of the second order on s-d hybridization, one gets four new currents: two additional ones for s-electron currents due to s-d hybridization at Cr|MgO and MgO/Fe interfaces and similarly the two for d-holes: $\Delta j^{s\uparrow}_2 + \Delta\tilde{j}^{s\uparrow}_2$, $\Delta j^{s\uparrow}_3 + \Delta\tilde{j}^{s\uparrow}_3$, $\Delta j^{d\downarrow}_2 + \Delta\tilde{j}^{d\downarrow}_2$, and $\Delta j^{d\downarrow}_3 + \Delta\tilde{j}^{d\downarrow}_3$. The detailed expressions for all corrections will be published elsewhere. Finally, the total current is given by the sum of all calculated zero order and additional integrated currents:

$$J_{\Sigma} = j^{\uparrow}_{0s} + j^{\downarrow}_{0d} + \Delta j^{s\uparrow}_2 + \Delta\tilde{j}^{s\uparrow}_2 + \Delta j^{s\uparrow}_3 + \Delta\tilde{j}^{s\uparrow}_3 + \Delta j^{d\downarrow}_2 + \Delta\tilde{j}^{d\downarrow}_2 + \Delta j^{d\downarrow}_3 + \Delta\tilde{j}^{d\downarrow}_3. \tag{6}$$

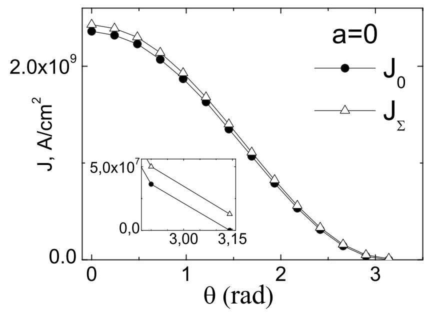

FIG. 1. Angular dependence of the current in Fe/MgO/Fe tunnel junction with no (j_0) and with s-d hybridization (j_Σ) taken into account. Inset shows a zoom around $\theta=\pi$.

III. RESULTS AND DISCUSSION

In order to demonstrate the impact of interfacial s-d hybridization using analytical results of the previous section, we calculated the angular dependence of both zero order and additional currents using Eqs. (4) and (6), respectively. The results of this calculation for Fe/MgO/Fe and Fe/Cr/MgO/Fe structures are shown in Figs. 1 and 2 with the parameters taken from Refs. 8 and 16. In Fig. 1 we show the dependence of the tunnel current across the standard Fe/MgO/Fe (Cr thickness $a=0$) junction as a function of angle between two Fe magnetizations. As one can see the tunnel current j_0 (filled circles) in the absence of s-d hybridization has usual angular dependence and vanishes for AP alignment of magnetizations ($\theta=\pi$) according to the half-metallic like picture according to our model with infinite TMR. At the same time, the total current j_Σ (open triangles) which takes into account the second order contributions due to s-d hybridization is not zero for AP configuration (see inset in Fig. 1). This happens because propagating majority (minority) s (d) electrons are converted at the interface into d (s) electrons and continues to propagate freely in the layer with opposite direction of the magnetization. The same dependences for the junction with finite Cr layer thickness are presented in Fig. 2. We notice a strong decrease in the parallel current value since the Cr represents an additional barrier for s-electrons (which is part of Δ_1 Bloch state). In addition, the role of s-d hybridization is further enhanced leading to significant drop of TMR ratio.

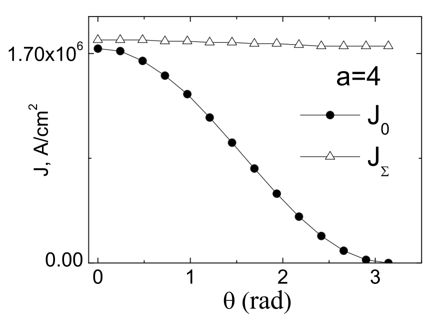

FIG. 2. The same dependencies as in Fig. 1 for Fe/Cr/MgO/Fe tunnel junction with finite Cr layer thickness.

We chose the model simulating the half metal nature for both s-electrons and d-electrons in the absence of hybridization to show more clearly the crucial influence of this hybridization on TMR. We have demonstrated that due to the s-d mixing the additional currents comparing with the incident s-up current appear. Due to these processes inside the barrier $j_d^\uparrow$ current even dominate the $j_s^\uparrow$ one because the $\psi_s^\uparrow$ states easily penetrate it. For the same reason in the region 3 in the vicinity of the interface the current $j_d^\downarrow$ almost defines the total current because s-electron on the interface transform in the d one, which according to the chosen half-metallic model easily propagates in the ferromagnetic.

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