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Tunneling Magnetoresistance of FeCo/MgO/FeCo Magnetic Tunnel Junctions

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Abstract

In this paper, tunneling magnetoresistance (TMR) of FeCo/MgO/FeCo magnetic tunnel junction (MTJ) is calculated theoretically using transfer matrix method. Band structure calculations are performed using ab initio Linearized Augmented Plane Wave (LAPW) method implemented in Wien2k program package. Fixed-spin moment (FSM) calculations are used to simulate the surface effects at the electrode/insulator interfaces which shows significant enhancement in polarization of the interfacial atoms of the electrodes. Our calculations show that for all cases taking the surface effects into account remarkably enhances the TMR of the MTJ.

Keywords: Magnetic tunnel junction, Tunneling magnetoresistance, Surface effects

1 Introduction

In recent years magnetic tunnel junctions (MTJs) have attracted great interest both due to the interesting physics behind them and their novel applications in areas such as spintronic scanning devices, magnetic sensors, and data storage technologies. Early MTJs were usually based on amorphous Al_2O_3 but theoretical investigation of transport properties of these tunnel junctions were predominantly limited to a model suggested by Jullière [1] which estimates the TMR of the junction from spin polarization of the electrodes. In these tunnel junctions, because of the amorphous nature of the barrier, a correct and unique specification of the electrode/insulator interface was almost impossible.

Later on TMRs of the order of a few 1000% was predicted in textured $FeCo_{1-x}/MgO/FeCo_{1-x}$ trilayers [2, 3]. It was discussed that this large magnetoresistance, very promising for the future spintronic applications, was achieved

due to a band matching at the electrode/barrier interfaces which led to an easier tunneling for one of the spin channels in comparison to the other. However, consequent experiments measured TMRs of around 300%, a value much smaller than the theoretically predicted TMR. These contrasting results between the theory and experiments led scientist to more severe investigations of the subject. Some suggested that during fabrication of the junction the electrode surfaces get oxidized and the oxidation hinders a perfect band matching at the interfaces. The calculations were repeated with the oxidation effect taken into account and the result was a 75% reduction in the calculated TMR for only 4% oxidation of the interface [4]. The oxidation effect was usually taken for one of the interfaces since during fabrication of the junction at the interface were MgO is going to be deposited onto the electrode because of their higher affinity the Oxygen atoms are more probable to bond to the surface electrode atoms [5]. Meyerheim et al. [6] suggest that surface oxidation of the electrodes can be avoided through simultaneous dosing with Mg to decrease the O/Mg ratio during the growth process. However, there are some experimental works which report absence of any oxidations at the interfaces [7].

2 Detailed Description of the Calculation Method

One of the simple methods for calculating the tunneling electric current in a ferromagnetic/insulator/ferromagnetic (FM/I/FM) tunnel junction is to approximate the electron wave functions within the electrodes with Bloch-like free electron wave functions and write the decaying wave function within the insulator as a combination of the Airy functions [8, 9]:

$$\psi_\sigma(x) = \begin{cases} A_{1\sigma}e^{ik_{1\sigma}x} + B_{1\sigma}e^{-ik_{1\sigma}x} & ; x < 0 \\ A_{2\sigma}\, Ai\left[\rho_\sigma(x)\right] + B_{2\sigma}\, Bi\left[\rho_\sigma(x)\right] & ; 0 < x < d \\ A_{3\sigma}e^{ik_{3\sigma}x} + B_{3\sigma}e^{-ik_{3\sigma}x} & ; x > d \end{cases} \tag{1}$$

where σ is denoting the electronic spin and d is thickness of the insulator. The unknown coefficients in Eq. 1 can be obtained via mutual matching of the wave functions and their derivatives at the interfaces. We assume a unit amplitude ($A_{1\sigma} = 1$) for the incident wave at the left side of the barrier and assume that there is no reflected wave at the right ($B_{3\sigma} = 0$). The wave vector within the electrodes as a function of energy of the incident electrons can be written as:

$$k_{1\sigma} = \sqrt{\frac{2m^*_{1\sigma}}{\hbar^2}\left(E - V_{1\sigma}\right)} \quad \& \quad k_{3\sigma} = \sqrt{\frac{2m^*_{3\sigma}}{\hbar^2}\left(E + V_a - V_{3\sigma}\right)} \tag{2}$$

where $m^*_{i\sigma}$ is the spin-dependent effective mass of the electrons, V_a is the applied bias, and $V_{i\sigma}$ is bottom of the energy band under consideration. Approximating the potential profile within a barrier of height U with a linear trapezoidal potential $V(x) = U - \frac{x}{d}V_a$ and solving the Schrodinger equation gives

$$\rho(x) = \frac{2m_2}{\hbar^2}\left(\frac{2m_2 \mathrm{V}_a}{\hbar^2 d}\right)^{-2/3}\left(U - E - \frac{x}{d}V_a\right) \tag{3}$$

for the argument of the Airy functions in Eq. 1.

Having calculated the wave function amplitudes in Eq. 1, the transmission coefficient across the barrier as a function of the energy and applied bias can be calculated through the relation

$$T_{\sigma\sigma'}(E, V_a) = \frac{m^*_{1\sigma}k_{3\sigma'}}{m^*_{3\sigma'}k_{1\sigma}}\left|\frac{A_3}{A_1}\right|^2 = \frac{4m^*_{1\sigma}k_{3\sigma'}}{m^*_{3\sigma'}k_{1\sigma}}\left|\frac{\delta_{\sigma'}Ai(d) - \gamma_{\sigma'}Bi(d)}{\alpha_\sigma\delta_{\sigma'} - \beta_\sigma\gamma_{\sigma'}}\right|^2 \tag{4}$$

where

$$\begin{cases} \alpha_\sigma = Ai(0) - \frac{im^*_{1\sigma}Ai'(0)}{m^*_2 k_{1\sigma}} \\ \beta_\sigma = Bi(0) - \frac{im^*_{1\sigma}Bi'(0)}{m^*_2 k_{1\sigma}} \\ \gamma_\sigma = Ai(d) + \frac{im^*_{3\sigma'}Ai'(d)}{m^*_2 k_{3\sigma'}} \\ \delta_\sigma = Bi(d) + \frac{im^*_{3\sigma'}Bi'(d)}{m^*_2 k_{3\sigma'}}\,. \end{cases} \tag{5}$$

Now the electric current for each channel can be calculated by integrating the transmission coefficient over the energy window determined from the electronic band structure of the electrodes,

$$I_{\sigma\sigma'}(V_a) = \frac{e_0 m^*_1 k_B T}{4\pi^2\hbar^3}\int_{E^{\min}_{\sigma\sigma'}}^{+\infty} T_{\sigma\sigma'}(E, V_a)\ln\left\{\frac{1 + \exp\left((E_F - E)/k_B T\right)}{1 + \exp\left((E_F - E - V_a)/k_B T\right)}\right\} dE \tag{6}$$

where k_B is the Boltzmann constant, T is the temperature, and $E^{\min}_{\sigma\sigma'} = \max(V_{1\sigma}, V_{3\sigma'} - V_a)$.

3 Results and Discussion

Here we consider a thin slab of MgO formed in NaCl crystal type sandwiched from sides by two FeCo electrodes. The electrodes have a $CsCl(B_2)$ type of crystal structure and thus in order to establish a connection between the two latices at the interfaces we had to rotate them by 45° with respect to each

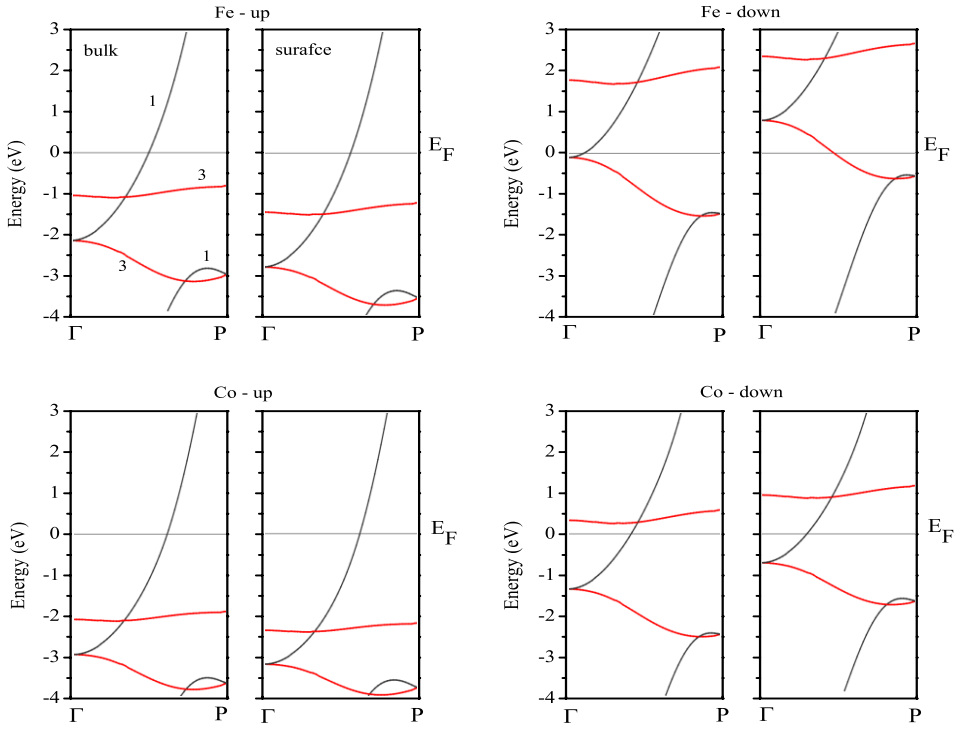

Figure 1: Bulk and surface spin-resolved band structure of the Fe and Co electrodes plotted in the Γ to P direction.

other. Our calculations were performed using the first-principle density functional theory in the framework of the FP-LAPW method [10] as implemented in the WIEN2k program package [11, 12, 13]. For the exchange-correlation potential, the generalized gradient approximation of Perdew-Berke-Ernzerhof [14] is applied. In separating the valence states from the core states, a separation energy of -7.0 and -8.0 Ry is used respectively for the Fe and Co atoms so as to take their 3s states as valence states [15]. Bulk volume optimized MgO lattice constants were calculated equal to 4.24 $\mathring{A}$. We have chosen the in-plane lattice constants of the electrodes equal to 2.94 $\mathring{A}$ which corresponds to an expansion of 2.6% in their lattice and a contraction of 1.9% in the MgO lattice.

In studying transport properties of MTJs it is very important to take the surface effects of the electrodes into account. According to our supercell calculations of the MTJ, the magnetic moment of the interfacial Fe atoms was calculated equal to $\sim 3.0\mu_B$ and that of the interfacial Co atoms was equal to $\sim 2.0\mu_B$ respectively for the Fe-ending and Co-ending electrodes. We simulated the surface effects using fixed-spin-moment calculations method [11]. Modifications in the energy bands of Fe and Co with inclusion of the surface

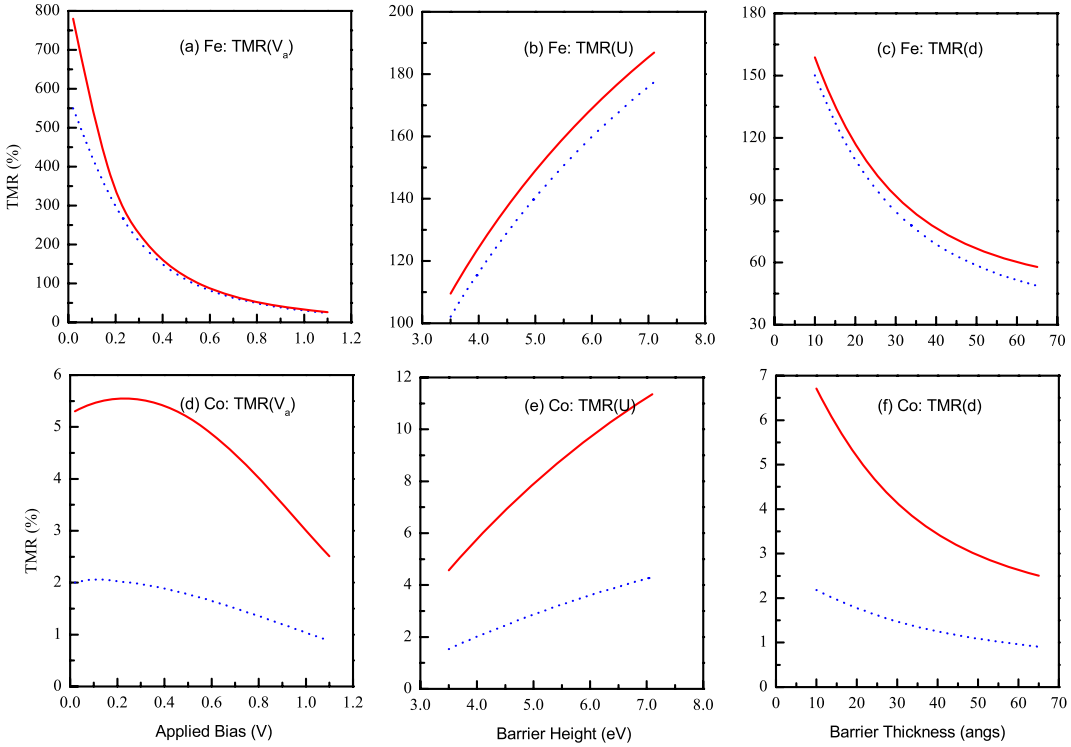

Figure 2: Tunneling magnetoresistance of the MTJ for the Fe and Co ending electrodes calculated as functions of the applied bias (V_a), barrier height (U), and the barrier thickness (d).

effects are depicted in Fig. 1 for both spins in the Γ to P direction. Almost a solid shift of the energy bands can be seen such that the spin-down Δ_1 band of Fe by moving above E_F gets totally depleted.

In the $\Gamma - P$ direction the only band which has significant contribution to the electron tunneling has the Δ_1 symmetry and other symmetries either don't find the corresponding symmetries at the interface to match with or decay so fast that their contribution can be ignored [2]. Using the energy bands in Fig. 1 we have calculated the electron effective masses of the Δ_1 band for using in Eqs. (2-6). The results are listed in Table 1.

Table 1: Spin-resolved electron effective masses of the Δ_1 bands of bcc Fe and Co along the $\Gamma - P$ direction.

	Fe		Co	
	$m^{*\uparrow}$	$m^{*\downarrow}$	$m^{*\uparrow}$	$m^{*\downarrow}$
bulk	$0.44m_0$	$0.42m_0$	$0.47m_0$	$0.48m_0$
surface	$0.43m_0$	$0.43m_0$	$0.46m_0$	$0.49m_0$

Fig. 2 presents results of the TMR calculations for the Fe and Co ending electrodes as functions of the applied bias, barrier height, and barrier thickness. In all cases inclusion of the surface effects enhances the TMR and for the case of Co the enhancement is remarkable. As expected for both Fe- and Co-ending interfaces the TMR decreases with increasing the applied bias (V_a) and the barrier thickness (d) and increases as the barrier height (U) increases. In panels (a) and (d) of Fig. 2 the barrier height and thickness are respectively set to 3.75 eV and 20 $\mathring{A}$. The parameters in panels (b) and (e) are $V_a = 0.5\ V$ and $d = 20\ \mathring{A}$ and in panels (c) and (f) they are set to $V_a = 0.5\ V$ and $U = 3.75\ eV$. Following Ref. [9] the effective mass of the Δ_1 band of MgO is chosen equal to $m_2^* = 0.35 m_0$.

4 Concluding Remarks

Using transfer matrix method we calculated tunneling magnetoresistance in FeCo/MgO/FeCo magnetic tunnel junction. We made a comparison between the TMRs of the Fe-ending and Co-ending electrodes and it was found out that the Fe-ending electrodes produce a much higher TMR. Band structure of the electrodes were calculated using DFT first-principles calculations and the fixed-spin-moment calculations were applied to simulate the surface effects at the electrode/insulator interfaces. The results are in range with the experimentally reported data. However, bringing into contact a metal with an insulator would induce some states, known as the metal induced gap states, within the energy gap of the interfacial layers of the interface which we have not taken into account in our calculations.

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