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S. Edalati Boostan and H. Moradi

Department of Physics, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran

E-mail: saeideh.edalati@gmail.com

Abstract.Tunneling magnetoresistance (TMR) is studied by using non-equilibrium Green's function method based on a single-band tight-binding approximation in Fe/MgO/Fe junction with random energy (RE) at interfaces. Roughness associated with interdiffused regions at Fe/MgO interfaces are introduced as RE on site elements of interfaces (atoms adjacent to interfaces). Calculations show that TMR and current density decrease in parallel configuration, but current density increases in anti-parallel configuration with roughness.

1. Introduction

TMR refers to an ultra-thin insulator sandwiched by two ferromagnetic (FM) electrode layers. The current density (J) through the tunnel barrier depends on the magnetization directions of the FMs when the directions are changed from being antiparallel (AP) to parallel (P) [1]. A larger magnetoresistance (MR) gives a more sensitive device which is desirable for great interest both for pure physics and device application [2]. The situation changed quite drastically with the recent observation of large values of TMR at room temperature (T) in junctions with an epitaxial MgO barrier [3, 4].The theories predict a MR ratio in excess of 1000% for ideal interfaces of Fe/MgO/Fe (001) [5-7]. This new development lends to understand the factors governing this effect, because the largest observed value 800% at low T and 472% at room T is still well below the theoretical values [5, 7]. Some effort has been devoted to explaining the discrepancy in terms of interface relaxation [8] or the formation of a layer of FeO at the interface [5, 9], and the role of interface disorder [10-12]. Disorder such as roughness at interface (RI) and lattice distortion might have a serious impact on TMR [11, 12]. Lattice disorder in the Fe layer can drastically reduce the TMR if the disordered layer is next to the barrier [13].

In this paper, we investigate how RI affects the J and TMR in Fe/MgO/Fe (100) junctions. In section 2, the model and the method to calculate the J of magnetic tunnel junctions (MTJs) are briefly explained. In section 3, the results are discussed, and the final section is summary.

2. The model and the method

In order to study transport properties in MTJs, it is important to take into account realistic interfaces. A schematic of device used for calculation is shown in figure 1. The figure1a shows ideal MTJ with

sharp interfaces and figure1b shows realistic MTJs with roughness at interfaces. The device is infinite in the transverse direction and has 8 layers in the longitudinal direction. We propose a theoretical method for Fe/MgO/Fe with RIs, based on a single-band tight-binding (SBTB) approximation [14]. We can use this method for any kind of MTJ materials and also for large systems due to its computational simplicity. For each $k_{\parallel}$, we have a 1D lattice. In SBTB each two atomic layers parallel with interface correspond to one unit cell and depicted by one point in 1D real lattice space as shown in figure 1c and 1d. In real world, due to diffusion of Fe and MgO, we don't have sharp interfaces. If some Fe (MgO) atoms adjacent to the MgO (Fe) layer are replaced by the MgO (Fe) atoms at interfaces, the voltage and consequently the on-site energies at interfaces change. Then, we introduce disorder in interfaces by random variations of thickness of layer, which then induce the fluctuations in the on-site atomic energies of width Δ within the Fe and MgO atoms adjacent to the interfaces. This method of introducing interface disorder within SBTB models is a well established approach [12,13]. Within more advanced models including ab intio methods more sophisticating treatments exist. One possibility is the supercell approach which is limited by the number of treatable configurations. The coherent potential approximation (CPA) is a self-consisting scheme to model substitutional disorder. For transport calculations using CPA the important vertex corrections have to be considered [11].
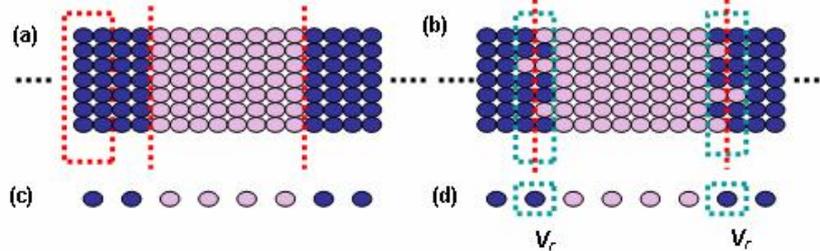

Figure1. MTJs in atomic scale for ideal MTJ with clean interfaces (a), and realistic MTJ with RIs (b). The dotted rectangular in (a) shows the unit cell and in (b) diffused interfaces. The dotted lines show sharp interfaces in ideal MTJs. In (c) and (d) each lattice point is as a unit cell in (a) and (b). (c) is real space lattice for ideal, and (d) realistic MTJs with random energies on-site adjacent to interfaces.

For the practical MTJs with symmetric RI, the device Hamiltonian in longitudinal direction is:

$$H_{SBTB} = \begin{cases} E_{bo} + 2t_o + U(i,j) + \Delta & i = j \\ -t_o & |i-j| = 1 \\ 0 & |i-j| > 1 \end{cases} \qquad (1)$$

where E_{bo}, t_O , $U(i, j)$ and Δ are band offset, hopping parameter, Laplacian potential and the width of distribution on-site atomic random energies of Fe and MgO atoms at interfaces with a uniform distribution, respectively(All the parameters are in ev). All Fe and MgO parameters are taken from the papers [15].

$$-V_r/2 \le \Delta \le V_r/2 \qquad\qquad V_r = 2 \qquad (2)$$

Δ refers to the randomness. The positive (negative) sign of Δ refers to replacement of MgO by Fe (Fe by MgO) atoms, and the magnitude of it shows how many of Fe (MgO) atoms are replaced by MgO (Fe). Applying an external bias voltage, V, the chemical potentials of the FMs μ_R (right) and $\mu_L = \mu_R + eV$ (left) are shifted with respect to each other. This means that the potentials and the corresponding bands are shifted. Due to the small transmission, we assumed a linear voltage drop inside the MgO barrier. Therefore, the ballistic J is

$$J^{\sigma} = \frac{e}{h} \int_{\mu_R}^{\mu_L} dE_L T^{\sigma}{}_{SBTB}[f_L - f_R] \qquad (3)$$

where f_L and f_R are the Fermi-Dirac functions for the left and right electrode, respectively. σ is the spin index standing for majority$\uparrow$ and minority$\downarrow$ spins. The transmission coefficient is given by

$$T^{\sigma}{}_{SBTB} = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \mathrm{d}k_x \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \mathrm{d}k_y T^{\sigma}(E_L) = \frac{1}{a^2} T^{\sigma}(E_L) \qquad (4)$$

where $a = 2.86$ Å is the Fe lattice constant. The transmission through the MTJs that obtained by the non-equilibrium Green's functions is given by $T^{\sigma}(E_L) = tr(\Gamma_1 G \Gamma_2 G^+)$. Here, $\Gamma_C = i(\Sigma_C - \Sigma_C^+)$ is the broadening matrix that describes the interaction of the scattering region energy levels with the left and right-hand side electrodes (c= 1, 2), and calculated by self-energies, $\Sigma_C = -t_O e^{-ik_{\parallel}a}$. $G(G^+)$ is the retarded (advanced) Green's function describing the one electron electronic structure of the scattering region. For each $k_{\parallel}$, Green's function is defined as:

$$G = [(E_L + i0^+)I - H_{SBTB} - \Sigma_C]^{-1} \qquad (5)$$

After identifying the configurational average of J in P (J_P) and AP (J_{AP}) configuration, TMR given by

$$TMR = \frac{J_P - J_{AP}}{J_{AP}} \qquad (6)$$

3. Results and Discussions

Figure 2 shows SBTB calculation of J for majority and minority electrons as a function of voltage for clean ($\Delta= 0$) and rough ($\Delta=2$) interfaces of Fe/MgO/Fe. Figure2a is for P and figure2b is for a AP configuration. Figure 2a shows that J of majority electrons in real junction especially in higher voltage ($\approx$1V) decreases compare to ideal junctions, but J of minority electrons shows a little increase. This shows that roughness increases (decreases a little) spin dispersion of majority (minority) electrons in P configuration. Figure2b indicates that in AP configuration, J of majority and minority electrons increase with roughness. This means that for both majority and minority electrons, roughness decreases spin dispersion. For minority electrons, in real junction the maximum value of J is about 0.5 V, and the roughness affects J of minority electrons a little (about in1 V).
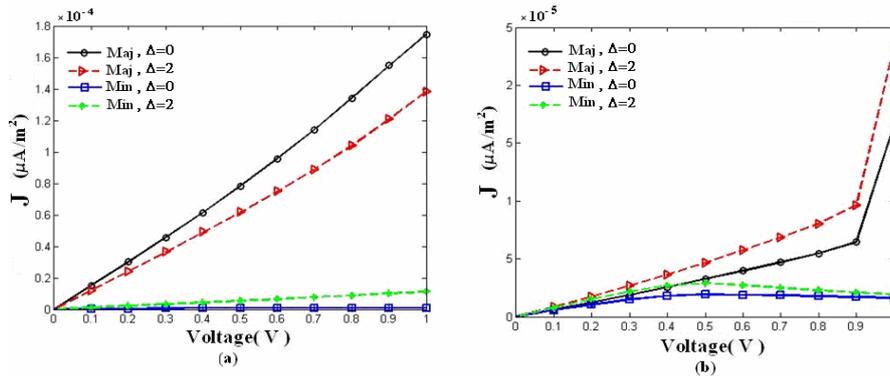

Figure2. J of majority and minority electrons are plotted as a function of voltage for clean (Δ=0) and rough (Δ=2) interfaces for P (a) and AP (b) configuration.

Figure3a shows J as a function of V in P and AP configurations for ideal (Δ =0) and realistic (Δ =2) MTJ. The plot shows that roughness decreases J_P while J_{AP} increases a little. This means that the total spin scattering of majority and minority electrons in P (AP) configuration increase (decrease) with roughness. This is probably due to change in the electronic levels at interfaces that provides additional

conduction channels for AP configuration and consequently increase J_{AP}, while presence of roughness in P configuration destroys the good matching between the band structure of Fe and MgO and causes a reduction in J_P. In addition, a dramatic increase in J_{AP} is observed in about 0.9 *V*. This is due to the change of the band structure. Figure3b shows TMR as a function of voltage for clean ($\Delta=0$) and rough ($\Delta=2$) interfaces. Then, according to figure3a, we expect the TMR decreases with roughness, figure3b. The other theories predict a very larger TMR than experimental observations [5, 7]. Then, the result of figure 3b is closer to experimental results.
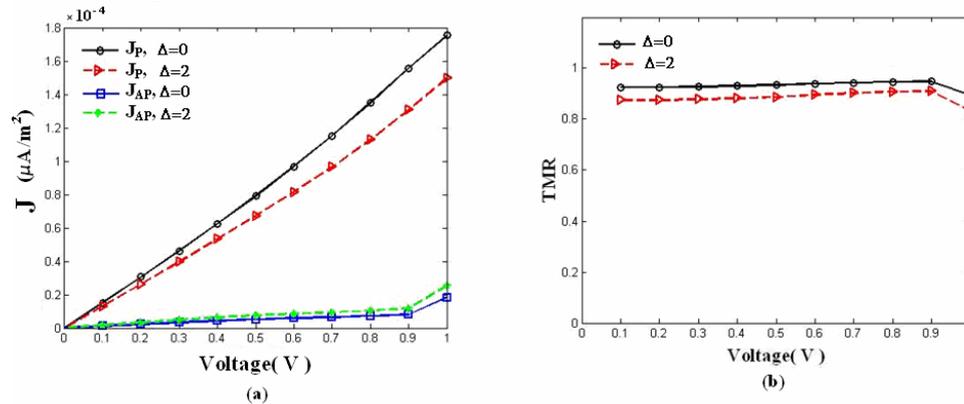

Figure3 (a) *J* is plotted as a function of voltage for ideal and real junctions. (b) TMR is plotted as a function of voltage for ideal and real junctions.

4. Summary

SBTB approximation and Green's function formalism was used to calculate the transport through Fe/MgO/Fe MTJ devices in [100] direction. We find that roughness decreases the current density in parallel configuration of ferromagnetic layers, but increases in antiparallel configuration in MTJ. Hence TMR reduces with roughness relative to ideal MTJ (without roughness) in good agreement with experimental results.

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