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Spin-polarized current and tunnel magnetoresistance in heterogeneous single-barrier magnetic tunnel junctions

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HIGHLIGHTS

- A model of heterogeneous tunnel junction is developed.
- The model takes into account Volta potential and the difference of effective masses.
- Calculations was done for Fe/MgO/Fe-like structures.
- It is shown the influence of the structure parameters on TMR.

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ABSTRACT

Current in heterogeneous tunnel junctions is studied in the framework of the parabolic conduction-band model. The developed model of the electron tunneling takes explicitly into account the difference of effective masses between ferromagnetic and insulating layers and between conduction subbands. Calculations for Fe/MgO/Fe-like structures have shown the essential impact of effective mass differences in regions (constituents) of the structure on the tunnel magnetoresistance of the junction.

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1. Introduction

Currently, layered magnetic nanostructures FM/I (ferromagnet/insulator) is one of the most exciting and rapidly developing areas of spintronics. Effects of tunneling magnetoresistance (TMR) and magnetization switching in such structures are used in magnetic field sensors, nonvolatile magnetoresistive memory (MRAM, ST-MRAM), resonant tunneling diodes, spin transistors [1,2,3]. In this report, I investigate theoretically the asymmetric (heterogeneous) one-barrier magnetic nanostructures $FM_L/I/FM_R$. They consist of two ferromagnetic metal layers separated by non-magnetic dielectric (insulating) layer. As a ferromagnetic layers material, Fe, Co, Ni and their alloys (CoFeB, FeNi) are considered. Insulating layer is usually AlO_x or MgO. Magnetization of one of the ferromagnetic layers (FM_L or FM_R) is pinned by exchange bias. Magnetization of the other layer can be changed by an external magnetic field.

Usually, one considers two situations referring to relative orientations of the ferromagnetic layer magnetizations. P-orientation (parallel) is referred to the case when magnetizations of the both ferromagnetic layers are parallel, AP-orientation (anti-parallel), when the magnetizations of the layers are directed opposite to each other. If we apply bias voltage to the external electrodes, a current flows across the structure. It is due to quantum mechanical tunneling of electrons through the barrier. Resistance of the structure depends on relative orientations of the ferromagnetic layers. The relative difference between resistances in the P and AP alignments may reach tens of percent at room temperature [4].

In early works the Julliere model [5] was used for description of the tunneling magnetoresistance in magnetic tunnel junctions (MTJ). This simple model considers TMR as a result of spin polarizations of the ferromagnetic electrodes. Slonczewski [6] further improved the Julliere model utilizing quasi-one-dimensional free electron model, however, the model could not predict negative TMR ratio at certain applied voltages that was obtained in experiment [7]. Similar approximations were made by Bratkovsky [8] (for half-metallic systems), and MacLaren [9] (comparison of

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Julliere and Slonczewski models). Zhang [10] calculated TMR for one- and double-barrier MTJ using one-dimensional Hamiltonian and Tsu-Esaki [11] formulas. The same approach was used by Wilczynski [12] and Khachaturov (using WKB-approximation for the transmission coefficient in FM-I-FM structures) [13]. Further, this approach was extended to the case of different effective masses in insulating and ferromagnetic layers ($m_{FM,L} = m_{FM,R} \neq m_I$) [14,15]. Montaigne [15] stressed that TMR behavior on voltage strongly depends on insulating layer parameters (effective mass of conducting electron, thickness and height of the barrier) and its asymmetry. This dependence was also shown in [16,17] (with addition of the image forces in the barrier region).

Here I report on results of investigation of the spin-dependent transport and tunnel magnetoresistance in heterogeneous (asymmetric, $FM_L \neq FM_R$) single-barrier magnetic tunnel junctions. As in the latest works cited above, I use free electron model and two parabolic subbands approximation for the conduction band of ferromagnetic layers. My model of the junction takes into account different effective electron masses in the ferromagnetic metals conduction subbands and the barrier as well, arbitrary widths of the spin-subbands and the barrier heights at the FM-I interface. Spin of the electron is conserved during tunneling trough the junction.

2. The model

For calculation of TMR, we need to derive formulas giving us the current density for every spin channel. The channels are shown schematically in Fig. 1. Each channel has its own width of the spin subbands and the effective masses in them. First, we will find a formula for the

current in the most general case, and then, apply it to the each spin channel. The tunnel magnetoresistance is given by the formula:

$$TMR = \frac{j^P - j^{AP}}{j^{AP}},$$
$$j^P = j_{\uparrow\uparrow} + j_{\downarrow\downarrow},$$
$$j^{AP} = j_{\uparrow\downarrow} + j_{\downarrow\uparrow}. \quad (1)$$

The potential profile in our case is shown in Fig. 2. It is assumed that thermodynamic equilibrium is reached, so that at zero voltage, the Fermi levels of the ferromagnetic electrodes are the same. U_1 and U_2 representing the height of the barrier imposed by the Volta potential (difference between work functions of the electrodes).

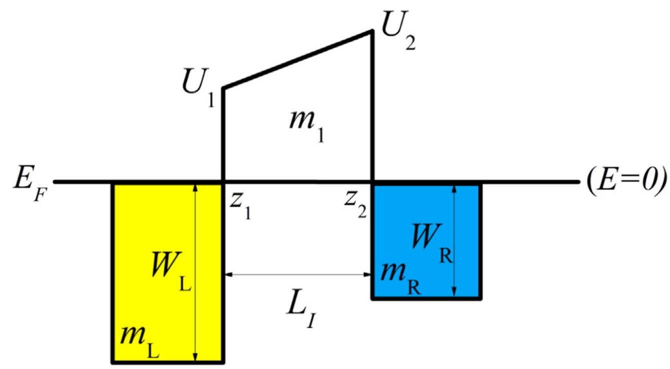

Fig. 2. Potential profile of the structure for the general case (at zero bias). W_L and W_R denote the widths of the subbands. m_L, m_I and m_R are the effective masses in the left, middle and right region respectively. U_1 and U_2 symbolize the barrier heights on the interfaces. The thickness of the middle layer is L_I.

The zero of energy is chosen at the Fermi level of the left electrode. Solving the Schrödinger equation in the FM layers for z-projection of the wave vectors we obtain:

$$k_{L,z} = \sqrt{\frac{2m_L}{\hbar^2}(E_z + W_L)},$$
$$k_{R,z} = \sqrt{\frac{2m_R}{\hbar^2}\left(E_z + E_{\parallel}\left(1 - \frac{m_L}{m_R}\right) + W_R + eV_a\right)}, \quad (2)$$

where $E_z = E - E_{\parallel}$, $E_{\parallel} = \hbar^2 k_{\parallel}^2 / 2m_L$, $k_{\parallel}^2 = k_x^2 + k_y^2$. The parallel wave vector is conserved in all regions because the potential energy of conduction electron depends only on z-coordinate. Following the approach described in [18], one can show that even for the heterogeneous case the general formula for the tunneling current density between conduction subbands of the electrodes in each spin-channel still keeps the conventional form (formula (2) in Ref. [19]):

$$j = \frac{e}{(2\pi)^3 \hbar} \iiint D(E_z, E_{\parallel})\left[f_L(E) - f_R(E)\right]\frac{\partial E}{\partial k_z} dk_x dk_y dk_z, \quad (3)$$

where $D(E_z, E_{\parallel})$ is the barrier transmission coefficient, and $f_L(E), f_R(E)$ are Fermi-Dirac functions of the left and right electrodes, respectively. Spin-channel indices are omitted for brevity. The factor of two according to Ref. [19], encountering two species of spin, is absent because Eq. (3) is written for one spin-channel of conduction.

Further, we proceed to integration from wave vectors to energy:

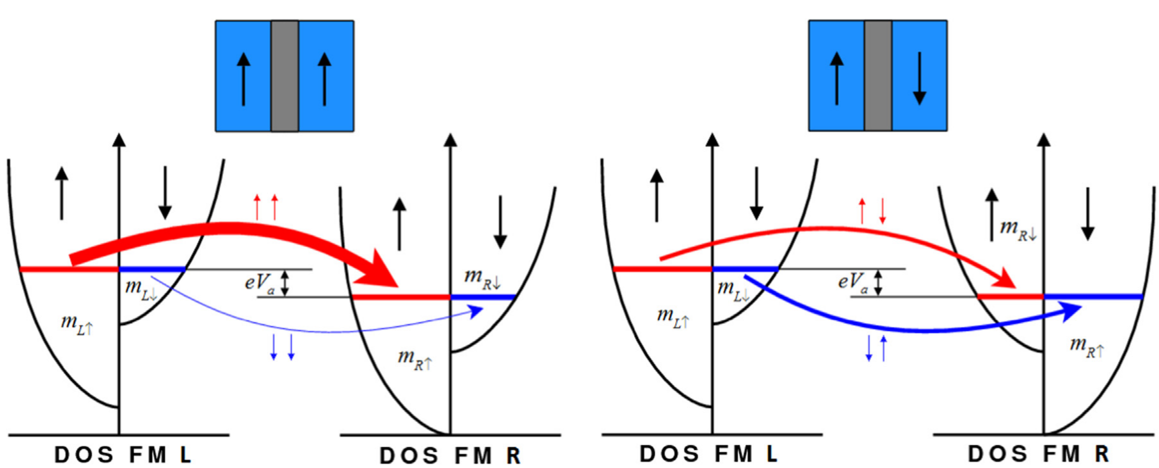

Fig. 1. Schematical view of the tunneling process between ferromagnetic subbands for P and AP configurations. On the top, the magnetizations of the layers are marked by black arrows. Colored arrows denote the conduction channels (majority-↑, minority-↓). Also are shown the effective masses and the applied voltage.

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