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Influence of a ZnO layer on Seebeck coefficients in asymmetric double-barrier tunnel junctions

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ABSTRACT

The Seebeck coefficients are studied in asymmetric double-barrier magnetic tunnel junctions (DBMTJs) with the structures as CoFeB/MgO/ZnO/MgO/LSMO. In the linear response regime, oscillatory behavior is observed with change in the ZnO layer thickness because of the resonant tunneling in the DBMTJs. Effects of average temperature and magnetizations orientation are also discussed. It is found that the Seebeck coefficients are greater in the DBMTJs than asymmetric single-barrier MTJs (SBMTJs). Therefore, it is to be achieved the greater Seebeck coefficients by choosing a proper thickness for the ZnO layer in the proposed asymmetric DBMTJs.

1. Introduction

Recently, thermoelectric (TE) topic have been attracted great attention in nano-structures [1,2]. Enhancement of TE effects are observed in nano-structures compared with bulk systems because of the localized states and phonon scattering [3,4]. The TE effects in magnetic tunnel junctions (MTJs) [5–8] are motivated by potential implementations in memory technologies [9]. The Seebeck coefficients have been shown different values in MTJs [5–8,10,11].

The energy conversion efficiency is described by dimensionless figure of merit as $ZT = S^2GT/\kappa$, where S denote the Seebeck coefficients, G the electrical conductance, the average temperature of the junction ($L(R)$: left (right) electrode) and κ thermal conductance at temperature T which is sum of the electronic contribution κ_e and phonon (lattice) contribution κ_p.

The localized states contribution to the Seebeck coefficients can be originated from quantum-well (QW) states in double-barrier MTJs (DBMTJs). The being of the QW states causes to the resonant tunneling (RT) in the DBMTJs which can be controlled by change the parameters such as the thicknesses of the QW layer and barriers, magnetic material type and so on. As a result, the Seebeck coefficients are much larger than those in single-barrier MTJs (SBMTJs). Recently, spin and charge thermopower of RT diodes [12], resonant enhancement in the TE performance [13] and power analysis of a RT diode [14] are studied theoretically. The Seebeck coefficients of the double tunnel junctions including spin-filter barriers [15] and the TE effects in the DBMTJs with middle ferromagnetic (FM) layer [16] are investigated.

ZnO is a semiconductor with a direct and wide band gap and it has a high exciton biding energy of $60meV$. Therefore, ZnO could be consider as a suitable candidate for applications in electronic and optoelectronic. MgO is an insulator with a simple rock-salt cubic structure as it looks an appropriate material for integrating with ZnO. As a result, grown of ZnO thin films on MgO (001) substrates are reported by several works [25–30].

Spin-transfer torque (STT) and thermal STT in asymmetric DBMTJs including a non-magnetic metal (NM) layer are studied recently [17,18]. However, the Seebeck coefficients in asymmetric DBMTJs with a ZnO layer have not been reported before.

The purpose of this paper is to discuss influence of a ZnO layer on the Seebeck coefficients in asymmetric DBMTJs with the structures as CoFeB/MgO/ZnO/MgO/LSMO (Fig. 1).

This paper is ordered as follows. Section 2 describes model and formalism. Results and discussion are presented in Section 3. Conclusions are explained in Section 4.

2. Model and formalism

A single-band effective mass Hamiltonian is considered as:

$$H = H_0 I - (\vec{\sigma}.\,\hat{m})\frac{\Delta}{2} \tag{1}$$

In the Hamiltonian, H_0 denote the spin-independent term, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ the Pauli spin vector, $\hat{m}$ the magnet direction and Δ the spin-splitting of the FM electrodes.

In the NEGF formalism [17–21], retarded Green's function G^r is given by:

$$G^r(E) = [EI - H - \Sigma_L^r - \Sigma_R^r]^{-1} \tag{2}$$

In Eq. (2), E symbolize the energy and $\Sigma_{L(R)}^r$ the left (right) retarded

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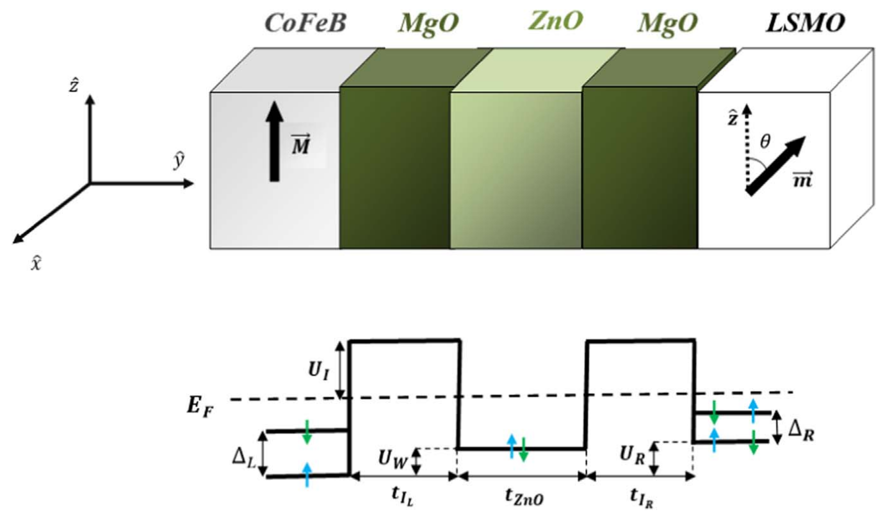

Fig. 1. Design of asymmetric double-barrier magnetic tunnel junctions (DBMTJs) with a ZnO layer. The magnetization of the CoFeB electrode is $\vec{M}$ along the z-axis and that of the LSMO electrode is $\vec{m}$ which it has an angle θ with the z-axis. The spin-splitting of the left electrode (CoFeB) is Δ_L and that of the right electrode (LSMO) is Δ_R. Symbols $t_{I_{L(R)}}$ and t_{ZnO} stand for the thickness of the left (right) insulator and ZnO layer, respectively. The barrier height of the insulator above the Fermi energy (E_F)is U_I. Difference in the conduction band of the CoFeB-ZnO is U_W and that of the CoFeB-LSMO is U_R.

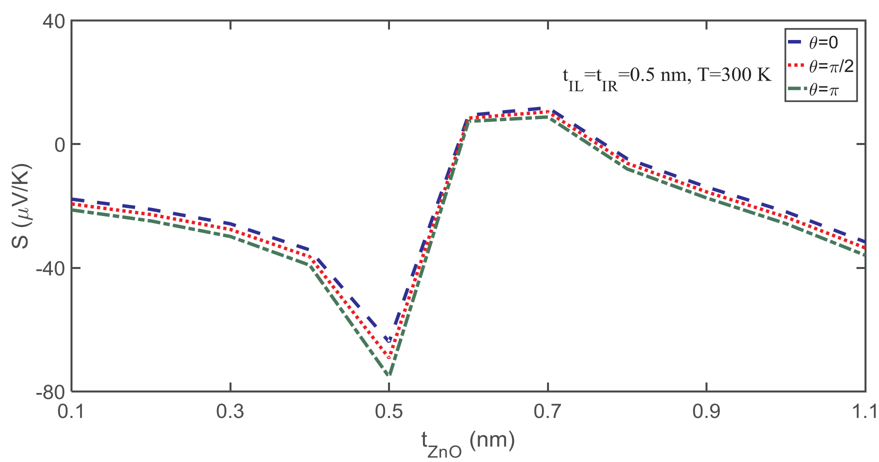

Fig. 2. Seebeck coefficients (S) as a function of the thickness of the ZnO layer (t_{ZnO}) with $t_{I_L} = t_{I_R} = 0.5nm$, $T = 300K$ and $\theta = 0, \pi/2, \pi$ in the asymmetric DBMTJs.

electrode self-energy matrix. Then the electronic transmission coefficient through the device is calculated as:

$$T_{trans}(E) = Tr\left[\Gamma^L(E)G^r(E)\Gamma^R(E)G^a(E)\right] \tag{3}$$

In Eq. (3), $G^a(E) = (G^r(E))^\dagger$ and $\Gamma^{L(R)}$ is the broadening matrix of the left (right) FM electrode which is given by:

$$\Gamma^{L(R)}(E) = i\left(\Sigma^{L(R)} - \Sigma^{L(R)^\dagger}\right) \tag{4}$$

A so small value of temperature difference $\Delta T = T_L - T_R$ is considered as the Seebeck coefficients are made in the linear response regime. Accordingly, the electric current I can be written as:

$$I = qL_0\Delta E_F + \frac{q}{T}L_1\Delta T \tag{5}$$

In Eq. (5), T denote the average temperature of the junction, q electron positive charge, the difference of the Fermi level locations in both electrodes corresponding to bias voltage ΔV made by the temperature gradient as $\Delta E_F = q\Delta V$ and ΔT the temperature difference of the FM electrodes.

The Seebeck coefficients (S) for zero current ($I \to 0$) are calculated using the following equation [22,23]:

$$S = \lim_{\Delta T \to 0}\left(\frac{\Delta V}{\Delta T}\right) = \left(\frac{k_B}{(-q)}\right)\frac{L_1}{L_0} \tag{6}$$

where

$$L_m = \int_{-\infty}^{+\infty}\left(\frac{E - E_F}{k_B T}\right)^m T_{trans}(E)\left(-\frac{\partial f}{\partial E}\right)dE \tag{7}$$

In Eqs. (6, 7), k_B denote the Boltzmann's constant and $f(E, T) = [e^{(E-E_F)/k_B T}+1]^{-1}$ the Fermi distribution function.

3. Results and discussions

The material parameters applied for the FM electrodes are the Fermi energy $E_F = 2.25eV$ [17,18,21], the effective mass for electrons inside the CoFeB electrode $m^*_{CoFeB} = 0.8m_e$ [17,18,21], the spin-splitting of the left (CoFeB) and right (LSMO) electrodes $\Delta_L = 2.15eV$ [17,18,21] and $\Delta_R = 0.7eV$ [17,18]. Difference in the conduction band of the CoFeB-LSMO is $U_R = 1.90eV$ and $m^*_{LSMO} = m^*_{CoFeB}$ [17,18], respectively. The material parameters applied for the MgO insulators, the ZnO layer are the barrier height of the insulators $U_I = 0.77eV$ [17,18,21], the effective mass for electrons inside the insulators $m^*_I = 0.18m_e$ [17,18,21], the effective mass for electrons inside the ZnO layer $m^*_{ZnO} = 0.29m_e$ [19] (