Theory of tunneling magnetoresistance and tunneling electroresistance in Co/BiFeO₃/La_{2/3}Sr_{1/3}MnO₃ junctions

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We present a theory of tunnel magnetoresistance (TMR) and tunnel electroresistance (TER) in multiferroic Co/BiFeO₃/La_{2/3}Sr_{1/3}MnO₃ junctions. Both the half-metallic band structure of the La_{2/3}Sr_{1/3}MnO₃ electrode and the multiferroicity in the BiFeO₃ barrier are considered explicitly in our model. Using transfer matrix method, we have derived an analytic formula for TMR in these structures. The calculations indicate that TMR is larger when the electric polarization in BiFeO₃ points to half-metallic La_{2/3}Sr_{1/3}MnO₃ and that the thicker the barrier is, the larger is the TMR, while for the negative electric polarization, the thicker the barrier is, the smaller is the TMR. In the mean time, the weak ferromagnetism, arising from spin-orbit coupling in BiFeO₃, is found to give a further variation of TMR and TER in these structures. These results agree with recent experimental observation well. © 2008 American Institute of Physics. [DOI: 10.1063/1.2974510]

I. INTRODUCTION

Magnetic tunnel junctions, i.e., structures composed of two ferromagnetic (FM) layers separated by a thin insulating barrier, have attracted great interest.^{1,2} The relative orientation of the magnetizations of two FM electrodes can affect dramatically the electron transport in such structures. This phenomenon gives rise to the so-called tunnel magnetoresistance (TMR).^{3,4} TMR is defined as $1 - R_P/R_{AP}$, where R_{AP} and R_P are the resistances of the junctions with antiparallel and parallel orientations of the magnetization in electrodes, respectively. The first understanding of TMR is the well known Julliere's formula $TMR = 2P^2/(1 + P^2)$,³ where P is the intrinsic spin polarization of electrodes. Most of the experiments have been carried out with Ni, Co, Fe, and their alloys as magnetic electrodes and an Al₂O₃ barrier; the observed TMR agrees with Julliere's formula.³

Significant TMR is beneficial for applications, and giant TMR was observed recently in Fe/MgO/Fe junctions. Besides the need for large TMR, electrically controllable functionality is also highly desirable.^{5,6} Multiferroics (MFs), where the spontaneous ferroelectric polarization can be controlled by an external magnetic field or vice versa, open the opportunity for novel spintronic devices.^{7–12} Strong ferroelectricity and large spontaneous electric polarization in BiFeO₃ thin films promise such electrically controllable functionalities.^{13–20} Junctions of Co/BiFeO₃/La_{2/3}Sr_{1/3}MnO₃ were prepared recently by Bea *et al.*^{21,22} It is assumed that unlike FM BiMnO₃ or La_{0.1}Bi_{0.9}MnO₃ based junctions,^{23–26} the spin filtering effect observed in FM BiMnO₃ or La_{0.1}Bi_{0.9}MnO₃ systems should be weaker in these antiferromagnetic (or weakly FM) BiFeO₃ systems. In fact, among the BiFeO₃ based junctions (with 2 or 5 nm thick BiFeO₃ barriers) prepared by Bea *et al.*, the maximum TMR is found

in a 5 nm case, the value of which reaches 31% but with signals that are a little noisy.²² In a stable 5 nm case, the TMR is 14%.²¹ This positive TMR reflects a positive spin polarization of $P_{Co} = 7.3\%$ if Julliere's formula [$TMR = 2P_1P_2/(1 + P_1P_2)$] and $P = 90\%$ for La_{2/3}Sr_{1/3}MnO₃ are invoked to explain this 14% TMR ratio.

For BiFeO₃ thin films, the thickness dependence of ferroelectric and FM properties is still controversial.^{13–20} It should be noted that ferroelectricity can be preserved down to 2 nm in BiFeO₃ epitaxial thin films.¹⁷ In the mean time, spin canting induced by spin-orbit coupling will give rise to weak ferromagnetism. The coexistence of ferroelectricity and ferromagnetism in the barrier has complicated the electron tunnel across Co/BiFeO₃/La_{2/3}Sr_{1/3}MnO₃ junctions. Moreover the experimental observations, i.e., the thickness dependence of TMR and the diversity of TMR ratio even for junctions with the same barrier's thickness, could not be explained either in Julliere's model,³ Slonczewski's model,⁴ or recent approaches.^{27–29}

The purpose of this paper is to give a clear picture of electron transport in these half-metallic MF junctions. The barrier's height, which is found to depend on the orientation of electric polarization; the barrier's thickness; the unique band structure of half-metallic La_{2/3}Sr_{1/3}MnO₃ electrode; and the spin filtering effect arising from spin canting in BiFeO₃ are considered explicitly in our transfer matrix calculations. In particular, a novel analytic TMR formula is obtained and the calculations agree with experiment well.

II. MODEL

A schematic illustration of the MF tunnel junction is shown in Fig. 1, with the unique band structure of half-metallic La_{2/3}Sr_{1/3}MnO₃ (Ref. 30) shown in Fig. 1(d). In particular, the multiferroism of the middle barrier, i.e., both the coexistence of electric polarization $\mathbf{P}$ and the FM exchange splitting, is considered, albeit in a somewhat simplified man-

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FIG. 1. (Color online) (a) Schematic illustration of MF tunnel junction. (b) Charge distribution and corresponding electrostatic potential. (c) The overall potential profile. (d) Schematic band structures of Co and half-metallic $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$.

ner. μ_L and μ_R are the Fermi energies of the left and the right electrodes. For the left and right FM electrodes and the MF barrier, the exchange splittings are Δ_L , Δ_R , and Δ_B , respectively. $U_L (=U_0 + \phi_L)$ and $U_R (=U_0 + \phi_R)$ are the electrostatic potentials at two interfaces relative to the Fermi level E_F of the system. The MF barrier is assumed to be uniformly electrically polarized and the effective barrier height $\bar{U}$ is $(U_L + U_R)/2$. The electric polarization $\mathbf{P}$ induces surface charge densities, $\pm\sigma_p = \pm|\mathbf{P} \cdot \mathbf{x}| = P \cos \alpha$, on the two surfaces of the barrier, where α is the relative orientation between the electric polarization $\mathbf{P}$ and the $\mathbf{x}$ axis. These polarization charges $\pm\sigma_p$ are screened by the screening charge per unit area, $\mp\sigma_s$, which is induced in the two metal electrodes. The MF barrier is assumed to be a perfect insulator and thus all the screening charge resides in the electrodes. According to the Thomas–Fermi model, the screening potential $\phi(x)$ is $\sigma_S \delta_L e^{-|x|/\delta_L/\epsilon_L}$ when $x \leq 0$ and is $-\sigma_S \delta_R e^{-|x-d|/\delta_R/\epsilon_R}$ when $x \geq d$.²⁷ Here, δ_L and δ_R are the Thomas–Fermi screening lengths in the left and right electrodes, respectively. ϵ_L and ϵ_R are the corresponding dielectric permittivities. The screening charge σ_S is obtained from the continuity of the electrostatic potential: $\sigma_S = (dP/\epsilon_B)/(\delta_L/\epsilon_L + \delta_R/\epsilon_R + d/\epsilon_B)$, where ϵ_B is the dielectric permittivity of the tunnel barrier.

Under the applied bias voltage V , the difference between the interfacial barrier heights is $\delta U = U_L - U_R = \delta\phi + eV$, where $U_L = \mu + \phi_L$ and $U_R = \mu + \phi_R - eV$. Letting $\mu = \mu_L$, the model Hamiltonian is given by

$$\hat{H}_\sigma = -\frac{\hbar^2}{2m_v} \nabla^2 + U(x) - \sigma_v \Delta_v \quad (v = L, B, \text{ or } R). \quad (1)$$

Here, $\sigma_v = \theta_v \sigma$ ($v = L, B, \text{ or } R$), where σ is the conserved spin orientation in three regions. $\sigma = +1(\uparrow)$ or $-1(\downarrow)$ means up-spin or down-spin with respect to the positive z direction. $\theta_v = +1(\uparrow)$ or $-1(\downarrow)$ denotes the magnetization direction in the region v , parallel or antiparallel to the positive z direction. Then $\sigma_v = +1(\uparrow)$ or $-1(\downarrow)$ is the relative spin orientation, parallel or antiparallel to the given magnetization in the region v . In the following calculation, we fix $\theta_R = +1(\uparrow)$, and let θ_B and θ_L vary.

Considering a spin-up incident plane wave from the left ferromagnet, the wave function in the left FM electrode is given by

$$\psi_L(x) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_\uparrow^\perp x} + R_\uparrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ik_\uparrow^\perp x} + R_\downarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ik_\downarrow^\perp x}, \quad (2)$$

where $R_\uparrow$ and $R_\downarrow$ are coefficients to be determined. In the barrier ($0 \leq x \leq d$), the wave is evanescent and has spin components

$$\psi_B(x) = A_\uparrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-\kappa_\uparrow^\perp x} + B_\uparrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{\kappa_\uparrow^\perp x} + A_\downarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-\kappa_\downarrow^\perp x} + B_\downarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{\kappa_\downarrow^\perp x}, \quad (3)$$

where $A_{\uparrow,\downarrow}$ and $B_{\uparrow,\downarrow}$ are coefficients. The right FM electrode has only the transmitted wave

$$\psi_R(x) = C_\uparrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_\uparrow^R(x-d)} + C_\downarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik_\downarrow^R(x-d)}, \quad (4)$$

with $C_{\uparrow,\downarrow}$ to be determined. To solve the Schrödinger equation, one must find the eight unknowns R_σ , A_σ , B_σ , and C_σ ($\sigma = \uparrow, \downarrow$) by matching ψ_σ and $d\psi_\sigma/dx$ at the interfaces $x = 0$ and $x = d$. The change in quantization axis at $x = d$ requires the spinor transformation matrix

$$\hat{T}_S = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & \sin\left(\frac{\theta}{2}\right) \\ -\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}, \quad (5)$$

where θ is the angle between the magnetizations of both FM electrodes. With the boundary conditions on the wave function, the above mentioned coefficients of the leading order in $e^{-\kappa_\uparrow^\perp d}$ and $e^{-\kappa_\downarrow^\perp d}$ are

$$R_\uparrow = A_\uparrow + B_\uparrow - 1,$$

$$R_\downarrow = A_\downarrow + B_\downarrow,$$

$$A_\uparrow = \frac{(\kappa_\uparrow + ik_\uparrow^\perp)B_\uparrow - 2ik_\uparrow^\perp}{\kappa_\uparrow - ik_\uparrow^\perp},$$

$$B_{\uparrow} = \frac{2k_{\uparrow}^L[2(\kappa_{\uparrow}\kappa_{\downarrow} + k_{\uparrow}^R k_{\downarrow}^R) - i(\kappa_{\uparrow} - \kappa_{\downarrow})(k_{\uparrow}^R + k_{\downarrow}^R) + i(\kappa_{\uparrow} + \kappa_{\downarrow})(k_{\uparrow}^R - k_{\downarrow}^R)\cos\theta]e^{-2\kappa_{\uparrow}d}}{(k_{\uparrow}^L + i\kappa_{\uparrow})[2(\kappa_{\uparrow}\kappa_{\downarrow} - k_{\uparrow}^R k_{\downarrow}^R) - i(\kappa_{\uparrow} + \kappa_{\downarrow})(k_{\uparrow}^R + k_{\downarrow}^R) + i(\kappa_{\uparrow} - \kappa_{\downarrow})(k_{\uparrow}^R - k_{\downarrow}^R)\cos\theta]}, \quad (6)$$

$$A_{\downarrow} = \frac{(\kappa_{\downarrow} + ik_{\downarrow}^L)B_{\downarrow}}{\kappa_{\downarrow} - ik_{\downarrow}^L},$$

$$B_{\downarrow} = \frac{8k_{\uparrow}^L\kappa_{\uparrow}(k_{\uparrow}^R - k_{\downarrow}^R)\sin\theta e^{-\kappa_{\uparrow}d}e^{-\kappa_{\downarrow}d}}{(k_{\uparrow}^L + i\kappa_{\uparrow})[2i(\kappa_{\uparrow}\kappa_{\downarrow} - k_{\uparrow}^R k_{\downarrow}^R) + (\kappa_{\uparrow} + \kappa_{\downarrow})(k_{\uparrow}^R + k_{\downarrow}^R) - i(\kappa_{\uparrow} - \kappa_{\downarrow})(k_{\uparrow}^R - k_{\downarrow}^R)\cos\theta]},$$

$$C_{\uparrow} = \frac{-8ik_{\uparrow}^L\kappa_{\uparrow}(\kappa_{\downarrow} - ik_{\downarrow}^R)\cos(\theta/2)e^{-\kappa_{\uparrow}d}}{(\kappa_{\uparrow} - ik_{\uparrow}^L)[2(\kappa_{\uparrow}\kappa_{\downarrow} - k_{\uparrow}^R k_{\downarrow}^R) - i(\kappa_{\uparrow} + \kappa_{\downarrow})(k_{\uparrow}^R + k_{\downarrow}^R) + i(\kappa_{\uparrow} - \kappa_{\downarrow})(k_{\uparrow}^R - k_{\downarrow}^R)\cos\theta]},$$

$$C_{\downarrow} = \frac{-8ik_{\uparrow}^L\kappa_{\uparrow}(\kappa_{\downarrow} - ik_{\downarrow}^R)\sin(\theta/2)e^{-\kappa_{\uparrow}d}}{(\kappa_{\uparrow} - ik_{\uparrow}^L)[2(\kappa_{\uparrow}\kappa_{\downarrow} - k_{\uparrow}^R k_{\downarrow}^R) - i(\kappa_{\uparrow} + \kappa_{\downarrow})(k_{\uparrow}^R + k_{\downarrow}^R) + i(\kappa_{\uparrow} - \kappa_{\downarrow})(k_{\uparrow}^R - k_{\downarrow}^R)\cos\theta]}.$$

The transmissivity $T = \text{Im}[\sum_{\sigma} \psi_{\sigma}^* (d\psi_{\sigma}/dx)]$ is obtained at $x = d^+$ for the cases of $\theta=0$ and π ,

$$T^{(0)} = \frac{16k_{\uparrow}^L k_{\uparrow}^R \kappa_{\uparrow}^2 e^{-2\kappa_{\uparrow}d}}{[\kappa_{\uparrow}^2 + (k_{\uparrow}^L)^2][\kappa_{\uparrow}^2 + (k_{\uparrow}^R)^2]}, \quad (7)$$

$$T^{(\pi)} = \frac{16k_{\downarrow}^L k_{\downarrow}^R \kappa_{\downarrow}^2 e^{-2\kappa_{\downarrow}d}}{[\kappa_{\downarrow}^2 + (k_{\downarrow}^L)^2][\kappa_{\downarrow}^2 + (k_{\downarrow}^R)^2]}.$$

For a small external voltage V , one can use the $V=0$ wave functions as shown in Eqs. (2)–(4). In the limit of the small barrier factor $e^{-2\kappa d}$, a narrow distribution of electrons near normal incidence and with E_x near E_F carry most of the current. Therefore $\kappa(E_x)$, $k_{\sigma}^L(E_x)$, and $k_{\sigma}^R(E_x)$ are replaced with $\kappa(E_F)$, $k_{\sigma}^L(E_F)$, and $k_{\sigma}^R(E_F)$, respectively:

$$k_{\sigma}^L = \lambda_L(E_F + \sigma\Delta_L)^{1/2}, \quad (8)$$

$$k_{\sigma}^R = \lambda_R(E_F - \Delta_E + \Delta_L - \Delta_R + \sigma\Delta_R)^{1/2}, \quad (9)$$

$$\kappa_{\sigma} = \lambda_B(\bar{U} - \sigma\Delta_B)^{1/2}. \quad (10)$$

Here $\lambda_v = \sqrt{2m_e^2/m_v\hbar^2}$ ($v=L, R$, and B), with m_e as the free-electron mass.

By summing the charge transmission over E_x and $\mathbf{k}_{\parallel}$ for occupied states, one finds $G_{\uparrow} = e^2\kappa_{\uparrow}T_{\uparrow}/8\pi^2\hbar d$, considering one initial spin direction, where e is the electron charge. When electrons with both values of σ are incident, the contribution of spin-down electrons should be added. Here, $T_{\uparrow}$ is given by Eq. (7) and $T_{\downarrow}$ is given by the same expression with $k_{\uparrow}^{L(R)}$ ($\kappa_{\uparrow}$) and $k_{\downarrow}^{L(R)}$ ($\kappa_{\downarrow}$) interchanged. We consider a FM/MF/FM tunnel junction in which all the momenta are real so that the two-band model is applicable to both ferromagnets. Four transmissivities $T_{\uparrow(\downarrow)}^{(0)}$ and $T_{\uparrow(\downarrow)}^{(\pi)}$ for both spin channels contribute to the parallel conductance $G^{(0)}$ and antiparallel conductance $G^{(\pi)}$, which are written as

$$G^{(0)} = G_{\uparrow}^{(0)} + G_{\downarrow}^{(0)} = \frac{2e^2}{\pi^2\hbar d} \left\{ \frac{16k_{\uparrow}^L k_{\uparrow}^R \kappa_{\uparrow}^2 e^{-2\kappa_{\uparrow}d}}{[\kappa_{\uparrow}^2 + (k_{\uparrow}^L)^2][\kappa_{\uparrow}^2 + (k_{\uparrow}^R)^2]} + \frac{16k_{\downarrow}^L k_{\downarrow}^R \kappa_{\downarrow}^2 e^{-2\kappa_{\downarrow}d}}{[\kappa_{\downarrow}^2 + (k_{\downarrow}^L)^2][\kappa_{\downarrow}^2 + (k_{\downarrow}^R)^2]} \right\}, \quad (11)$$

$$G^{(\pi)} = G_{\uparrow}^{(\pi)} + G_{\downarrow}^{(\pi)} = \frac{2e^2}{\pi^2\hbar d} \left\{ \frac{16k_{\downarrow}^L k_{\downarrow}^R \kappa_{\downarrow}^2 e^{-2\kappa_{\downarrow}d}}{[\kappa_{\downarrow}^2 + (k_{\downarrow}^L)^2][\kappa_{\downarrow}^2 + (k_{\downarrow}^R)^2]} + \frac{16k_{\uparrow}^L k_{\uparrow}^R \kappa_{\uparrow}^2 e^{-2\kappa_{\uparrow}d}}{[\kappa_{\uparrow}^2 + (k_{\uparrow}^L)^2][\kappa_{\uparrow}^2 + (k_{\uparrow}^R)^2]} \right\}.$$

Let us consider two special cases. When the right electrode is a half metal and the left one is a conventional FM metal, $k_{\uparrow}^R$ is imaginary and both $G_{\uparrow}^{(0)}$ and $G_{\uparrow}^{(\pi)}$ vanish. Thus

$$\text{TMR} = 1 - \frac{G_{\uparrow}^{(\pi)}}{G_{\uparrow}^{(0)}} = \frac{2P_L}{1 + P_L}, \quad (12)$$

where

$$P_L = \frac{Ak_{\uparrow}^L - Bk_{\downarrow}^L}{Ak_{\uparrow}^L + Bk_{\downarrow}^L} \quad (13)$$

is the effective spin polarization of the left FM electrode, with

$$A = \kappa_{\uparrow}^2 + (k_{\downarrow}^L)^2 \quad (14)$$

and

$$B = \kappa_{\downarrow}^2 + (k_{\uparrow}^L)^2. \quad (15)$$

On the other hand, when the left electrode is half metallic, the corresponding TMR is

$$\text{TMR} = 1 - \frac{G_{\downarrow}^{(\pi)}}{G_{\downarrow}^{(0)}} = \frac{2P_R}{1 + P_R}. \quad (16)$$

Here

$$P_R = \frac{Ck_{\uparrow}^R - Dk_{\downarrow}^R}{Ck_{\uparrow}^R + Dk_{\downarrow}^R}, \quad (17)$$

with

$$C = \kappa_{\uparrow}^3 [\kappa_{\downarrow}^2 + (k_{\uparrow}^L)^2] [\kappa_{\downarrow}^2 + (k_{\downarrow}^R)^2] e^{-2\kappa_{\uparrow} d} \quad (18)$$

and

$$D = \kappa_{\downarrow}^3 [\kappa_{\uparrow}^2 + (k_{\downarrow}^L)^2] [\kappa_{\uparrow}^2 + (k_{\downarrow}^R)^2] e^{-2\kappa_{\downarrow} d}. \quad (19)$$

With the above consideration, for a general case, the analytical TMR formula is

$$\text{TMR} = \frac{2P_L P_R}{1 + P_L P_R}, \quad (20)$$

where the barrier properties, i.e., effective barrier height $\bar{U}$; the exchange splitting of the barrier, Δ_B ; and the electric polarization in the barrier, $\mathbf{P}$, are included completely in the effective extrinsic spin polarizations P_L and P_R as described above [Eqs. (13) and (17)].

It is noted that in original Julliere's formula,³

$$\text{TMR} = \frac{2P^2}{1 + P^2}, \quad (21)$$

the spin polarization $P = (N_{\uparrow} - N_{\downarrow}) / (N_{\uparrow} + N_{\downarrow})$ and N is the density of states at Fermi level. On the other hand, in the model by Slonczewski,⁴ the barrier height on the tunneling is considered and $P = [(k_{\uparrow} - k_{\downarrow}) / (k_{\uparrow} + k_{\downarrow})] [(\kappa^2 - k_{\uparrow} k_{\downarrow}) / (\kappa^2 + k_{\uparrow} k_{\downarrow})]$, where $\kappa = \sqrt{(2m/\hbar^2)(U - E_F)}$ and U is the height of barrier. In the MF tunnel junction we study in this paper, the multiferroism has been included in the effective spin polarization for the first time.

For the MF half-metallic junctions (e.g., the Co/BiFeO₃/La_{2/3}Sr_{1/3}MnO₃ structure in Ref. 21) we considered in this paper, the large electric polarization $\mathbf{P}$ in BiFeO₃ and the half metallicity of La_{2/3}Sr_{1/3}MnO₃ can be considered explicitly in the above framework [as shown in Fig. 1(d)]. Moreover

$$\text{TMR} = 1 - \frac{k_{\perp}^L}{k_{\uparrow}^L} \left[1 + \frac{(k_{\uparrow}^L)^2 - (k_{\downarrow}^L)^2}{\lambda_B^2 (U_0 - \Delta_B + P \cos \alpha) (k_{\uparrow}^L)^2} \right], \quad (22)$$

where

$$t = \frac{\frac{d}{2\epsilon_B} \left(\frac{\delta_L}{\epsilon_L} - \frac{\delta_R}{\epsilon_R} \right)}{\frac{\delta_L}{\epsilon_L} + \frac{\delta_R}{\epsilon_R} + \frac{d}{\epsilon_B}}. \quad (23)$$

III. RESULTS AND DISCUSSION

First, we note that in both the models of Julliere³ and Slonczewski,⁴ neither the electric polarization nor the magnetism of the barrier was considered. Therefore, to appreciate the main finding of our model, we plot the TMR from Eq. (22) as a function of the orientation of the electric polarization in Fig. 2. Clearly, the orientation of the electric polarization has a rather strong influence on the magnitude of the TMR from Eq. (22) (see Fig. 2). Furthermore, Slonczewski's model⁴ is a special case of our Eq. (22) with $\mathbf{P} = 0$ (or $\alpha = 0$)

FIG. 2. (Color online) The electric polarization orientation (α) dependence of the TMR from Eq. (22). The TMR from both Julliere's and Slonczewski's models is α independent. The parameters used are the same as that used in the calculations in Fig. 3. Here a 5 nm thick nonmagnetic barrier is adopted.

and $\Delta_B = 0$. We also note that the difference in the TMR between Slonczewski's and Julliere's formulas is due to the fact that the barrier's height U_0 is not considered in Julliere's model.^{3,4}

In Figs. 3(a) and 3(b), we show the orientation dependence of conductance (with parallel magnetizations in two electrodes, G_P , and with antiparallel magnetizations in two electrodes, G_{AP}) and the TMRs for three junctions with thicknesses of 2, 3.5, and 5 nm, respectively. TMR decreases when $\mathbf{P}$ is reversed from the right to the left. When $\mathbf{P}$ points to the right, the thicker the barrier is, the larger is the TMR. However, when $\mathbf{P}$ is reversed, the thicker the barrier is, the smaller is the TMR. These results explain the diversity of TMR ratios observed in junctions even with the same d . It is also noted that the thickness dependence of TMR is quite

FIG. 3. (Color online) (a) The orientation of electric polarization (α) dependence of conductance. (b) α dependence of TMR. (c) The exchange splitting of the barrier (Δ_B) vs conductance. (d) Δ_B vs TMR. (e) α dependence of the normalized conductance $G(\alpha)/G(\alpha=0)$ with parallel magnetization in two electrodes. (f) Δ_B dependence of TER with parallel (P) and antiparallel (AP) magnetizations in two electrodes.

different from previously studied spin filter junctions, where the TMR shows a monotonic increase as the barrier's thickness increases.^{23–25,29} The reason is that the half-metallic band structure of $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ electrode is considered explicitly in our model and so there is only a spin-up electron transport channel. The parameters used here are from experiments or first principles calculations, i.e., half-metallic band structure of $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$,^{30,31} $\Delta_L=0.8$ eV for Co,³² band gap $U_0=2$ eV for BiFeO_3 ,³³ and $P=100$ $\mu\text{C}/\text{cm}^2$ for BiFeO_3 .³³ $\delta_R=0.07$ Å and $\delta_L=1$ nm, which are consistent with the results in Ref. 34. Despite the experimental controversy on the issue whether BiFeO_3 thin films can possess ferromagnetism,^{13–20} theoretically, first principles calculations indicate that spin-orbit coupling will give rise to spin canting, i.e., weak ferromagnetism.³⁵ This weak ferromagnetism may result in spin filtering effects on TMR by producing nonzero Δ_B . The negative Δ_B means that the orientation of magnetization in barrier is antiparallel to the magnetization in the right electrode. In Figs. 3(c) and 3(d), we show the Δ_B dependences of conductance (G_P and G_{AP}) and TMR, respectively. One can find that TMR decreases significantly with the increase in exchange splitting. This result suggests that the experimentally observed 31% (or less) TMR in $\text{Co}/\text{BiFeO}_3/\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ junctions^{21,22} may be due to the weak ferromagnetism of the barrier.

Lastly, we predict the change in conductance when an electric field is applied to rotate the orientation of $\mathbf{P}$ in BiFeO_3 . Since both electrodes and barrier are ferromagnetic, such tunnel electroresistance (TER),

$$\text{TER} = \frac{G(\pi)}{G(\alpha=0)}, \quad (24)$$

is a little different from that in a previously studied case in ferroelectric tunneling junctions.^{27,28} In Fig. 3(e), we show such TER as for junctions with various barrier thicknesses. It is found that TER increases with the increase in d and when the magnetization of the barrier is parallel to the magnetization of right electrode, the presence of weak ferromagnetism in BiFeO_3 will make TER more significant [Fig. 3(f)]. However, it is also noted that TER is almost independent of the magnetic configuration of two electrodes, i.e., parallel or antiparallel. These TER effects will be studied experimentally by Bea *et al.*^{21,22}

It should be noted that in our simple model we consider only the general aspects of half-metallic MF junctions (the half-metallic band structure of electrode and the exchange splitting and ferroelectric polarization of MF barrier) and the results are qualitatively valid. The detailed band structure of specific barrier and electrode (e.g., antiferromagnetic BiFeO_3 or FM BiMnO_3), the charge distribution and chemical bonding at certain interfaces, and the magnetoelectric coupling in specific MFs can be considered explicitly in future first principles calculations. The rapid decay of TMR in $\text{Co}/\text{BiFeO}_3/\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ junctions as a function of temperature is similar to that in other doped manganite based tunnel junctions and can be understood as a result of rapid decrease in spin polarization in the half-metallic $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ electrode, where the surface states are found to be quite different from those of the bulk.³⁶

IV. SUMMARY

In summary, we have presented a theory of TMR and TER in half-metallic MF $\text{Co}/\text{BiFeO}_3/\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ structures. We have explicitly considered the effects of electric polarization in BiFeO_3 and the unique band structure of half-metallic $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ in our simple model. Transfer matrix calculations indicate that TMR depends strongly on the orientation of electric polarization in BiFeO_3 and on BiFeO_3 's thickness. In the mean time, spin filtering effect, arising from the weak ferromagnetism of BiFeO_3 , is found to give a further variation of TMR and TER. Our findings not only explain recent experimental observations but also predict giant electroresistance when the electric polarization is reversed in these structures.

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