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Theoretical study on the positive magnetoresistance in perovskite oxide *p*–*n* junctions

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ABSTRACT

Taking spin current into account, the dependence of magnetoresistance with negative bias and that with doping concentration with various spin polarization in $La_{0.9}Sr_{0.1}MnO_3/SrNb_{0.01}Ti_{0.99}O_3$ *p*–*n* junction are obtained theoretically. The variation of the magnetoresistance value with the reverse bias is found to be due to the competition between the tunneling rate of electrons in $e_g^1\uparrow$ band at the homogeneous region of $La_{0.9}Sr_{0.1}MnO_3$to $t_{2g}\downarrow$ band and that to $e_g^2\uparrow$ band at the interface region of $La_{0.9}Sr_{0.1}MnO_3$. From the comparison of calculated magnetoresistance and the experimental data, a dependence of spin polarization of the system on the applied magnetic field is obtained.

Much attention has been focused on perovskite oxide owing to its nearly 100% spin polarization in ferromagnetic state and therefore, the perovskite oxide is a good candidate for devices using spin polarized charge transport [1–7]. Furthermore, in perovskite oxides the interface effect can cause polarization enhancement [8], superconductivity [9], a high-mobility electron gas [10] and positive magnetoresistance [11]. In spite of the multiple couplings among charge, spin and orbital degrees of freedom in the perovskite oxide, the transport behavior in perovskite oxide *p*–*n* junctions can be explained as the drift-diffusion mechanism in the positive bias and tunneling mechanism in the reverse bias condition with the consideration of oxide vacancies [12–14]. Positive magnetoresistance is found in many heterostructures with different materials [15–20]. In the perovskite oxide *p*–*n* junction composed of hole doped $La_{0.9}Sr_{0.1}MnO_3$ (LSMO) with negative magnetoresistance and electron doped nonmagnetic $SrNb_{0.01}Ti_{0.99}O_3$ (SNTO) the positive colossal magnetoresistance (CMR) effect is found [21,22]. The combination of all these issues is what makes oxide heterostructures so interesting: This area of research is located at the intersection between fundamental science investigations and technological applications [23]. Although the positive CMR effect is found in LSMO/SNTO heterojunction in the experiment and the origin of the positive CMR effect is proposed [11], the theoretical proof on the mechanism of positive MR and a quantitative calculation is still absent so far.

In this work, spin polarization is first employed in the transport calculation of perovskite oxide *p*–*n* junctions. Calculations for the tunneling spin currents are carried out at reverse bias by solving Schrödinger equation. The good agreement between the experimental and calculated results proves that the employment of spin current is valid to reveal the mechanism of positive MR behavior in the perovskite oxide *p*–*n* junctions. Furthermore, this method should be useful for designing MR-dependent devices in perovskite oxides.

Based on the drift-diffusion model, the energy band diagram, which is the basis for calculating tunneling current, is obtained [12–14]. Fig. 1 shows the calculated band structure around the interface regions of LSMO and SNTO *p*–*n* heterostructures at bias −0.5 V. Moreover, the schematic DOS (density of states) of the *p*–*n* junction is also plotted in Fig. 1. The tunneling current is calculated as follows: in the energy range from E_{fn} (the Fermi level in the SNTO) to E_{vp} (the top of the valence band in the left boundary of LSMO), the electron in the valence band of bulk LSMO region can tunnel to the conduction band in the space charge region of LSMO and SNTO. The wave function is obtained by solving Schrödinger equation in one dimension which is expressed as $-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2}+V(x)\varphi(x)=E\varphi(x)$, where $\hbar$ is reduced Planck's constant, m is effective mass of electron, $\varphi(x)$ is wave function, $V(x)$ is

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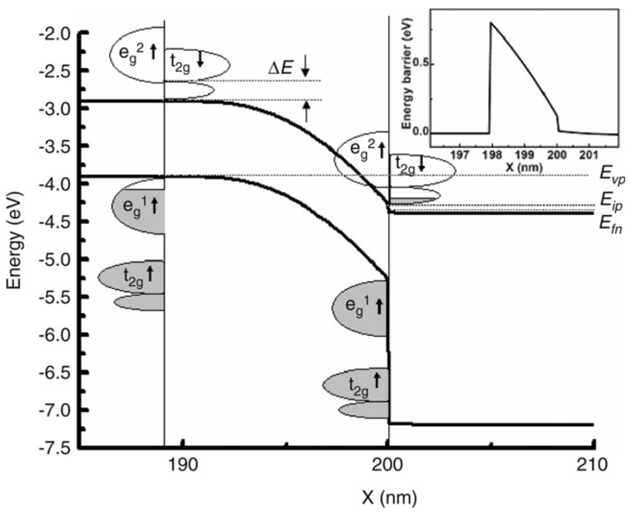

Fig. 1. The energy band structure at −0.5 V bias with the electron and hole doping concentration 2.0 × 10^{20} cm^{-3} for SNTO and 4.0 × 10^{19} cm^{-3} for LSMO respectively at 255 K in LSMO/SNTO junction and the corresponding schematic DOS of the junction. The inset shows the energy barrier at the space charge region of LSMO/SNTO junction.

the energy barrier, which is shown in the inset of Fig. 1, has been obtained by solving Poisson equation and the carrier continuity equations self-consistently, E is the energy of electron at a given energy. The Schrödinger equation is calculated by the finite difference discrete method. The free electron wave function is used as incident wave function, the wave function before entering the energy barrier is the sum of the incident and reflective wave function and after tunneling through the energy barrier, the wave function is the transmission wave function. And then the current density of a single electron $j_0(E) = \frac{i\hbar}{2m}(\varphi(x)\frac{d\varphi^*(x)}{dx} - \varphi^*(x)\frac{d\varphi(x)}{dx})$ can be obtained. The total current density is calculated using the expression in the following $J(0) = \int_{E_{fn}}^{E_{vp}} f(E)N(E)j_0(E)dE$, with $f(E) = \frac{1}{1+\exp\left(\frac{E-E_{fn}}{k_BT}\right)}$ being Fermi distribution function, $N(E)$ being the energy density of states of electrons taken as three-dimensional one, E_{fn} and E_{vp} being taken from our previous calculations [12–14], k_B and T being Boltzmann constant and temperature, respectively. The current density in the forward is two orders of magnitude larger than that in the reverse. Therefore, the current density in the reverse is omitted in our work.

At a given negative bias, if the energy difference between E_{ip} (the bottom of conduction band of LSMO at the interface) and E_{vp} is less than ΔE (the energy difference shown in Fig. 1), the expression for spin-dependent tunneling current density under magnetic field can be written as: $J_{\uparrow\to\downarrow}(P) = \int_{E_{ip}}^{E_{vp}} 0.5(1-P)f(E)N(E)j_0(E)dE$, where P is the spin polarization defined as $P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$, $N_\sigma(\sigma = \uparrow, \downarrow)$ are spin-dependent density of states for electrons with spin σ. When the energy difference between E_{ip} and E_{vp} is larger than ΔE, the expressions for spin-dependent tunneling current densities under magnetic field are:

$$J_{\uparrow\to\downarrow}(P) = \int_{E_{ip}}^{E_{vp}} 0.5(1-P)f(E)N(E)j_0(E)dE, \quad \text{and}$$

$$J_{\uparrow\to\uparrow}(P) = \int_{E_{ip}+\Delta E}^{E_{vp}} 0.5(1+P)f(E)N(E)j_0(E)dE.$$

$J_{\uparrow\to\downarrow}$ and $J_{\uparrow\to\uparrow}$ denote spin-related tunneling current densities of electrons in e_g^1 ↑ band to t_{2g} ↓ band and to e_g^2 ↑ band, respectively. The total tunneling spin current can be expressed as:

$$J(P) = J_{non} + J_{\uparrow\to\downarrow}(P) + J_{\uparrow\to\uparrow}(P), \tag{1}$$

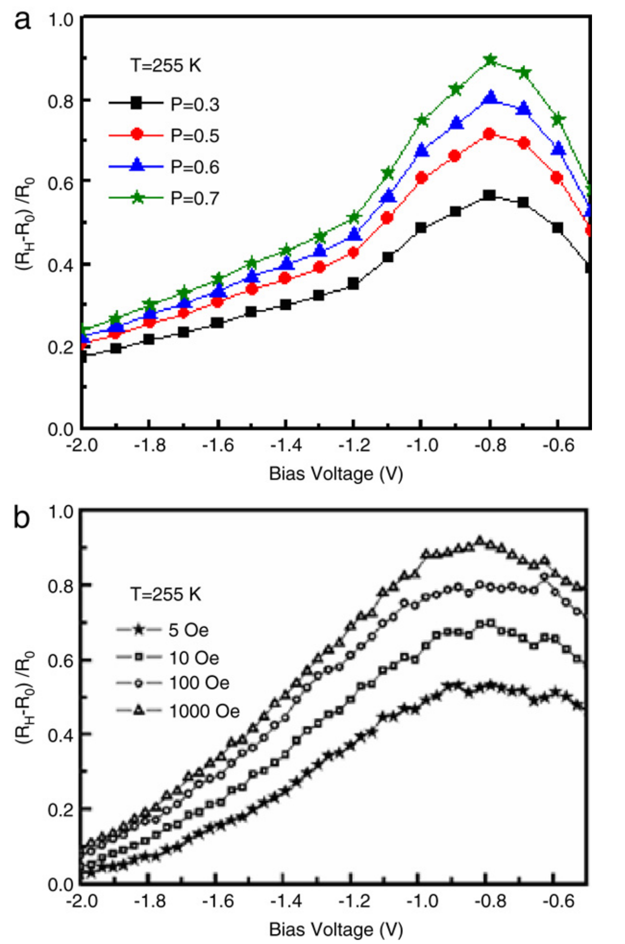

Fig. 2. (a) The calculated results of MR value dependent on negative bias at spin polarization 0.3, 0.5, 0.6, and 0.7 at the temperature of 255 K in LSMO/SNTO junction. (b) The experimental data of MR value dependence on negative bias under the magnetic field of 5 Oe, 10 Oe, 100 Oe and 1000 Oe at 255 K in LSMO/SNTO junction.

where $J_{non} = \int_{E_{fn}}^{E_{ip}} f(E)N(E)j_0(E)dE$, for clearly analyzing our later results of MR variation, the current for $P = 0$, $J(0)$ can be further written as $J(0) = J(P) + J_2(P)$, where $J_2(P) = \int_{E_{ip}}^{E_{vp}} 0.5(1+P)f(E)N(E)j_0(E)dE$, or $J_2(P) = \int_{E_{ip}}^{E_{ip}+\Delta E} 0.5(1+P)f(E)N(E)j_0(E)dE$, for the energy difference between E_{ip} and E_{vp} being less or more than ΔE, respectively. The MR is defined as $MR = (R_H - R_0)/R_0$, with the resistances under applied magnetic field $R_H = \frac{V}{I(P)}$ and zero magnetic field $R_0 = \frac{V}{I(0)}$ calculated with the calculated tunneling currents and applied bias, so that the expression for MR can be written as:

$$MR = \frac{J_2(P)}{J(P)}, \tag{2}$$

Fig. 2(a) shows the calculated MR value dependence on negative bias for spin polarization of 0.3, 0.5, 0.6, and 0.7, respectively, at the temperature of 255 K in LSMO/SNTO p–n junction. The corresponding experimental results are shown in Fig. 2(b) [11]. From the dependence of MR value with reverse bias with various spin polarization, it can be seen that with the increase of reverse bias, the value of MR increases to a maximum and then decreases swiftly. Furthermore, it increases with spin polarization at a given negative bias. From the comparison of Fig. 2(a) with (b), it can be seen that spin polarization of the structure increases with magnetic field and the calculated results are in good agreement with experimental data. At a small negative bias under magnetic

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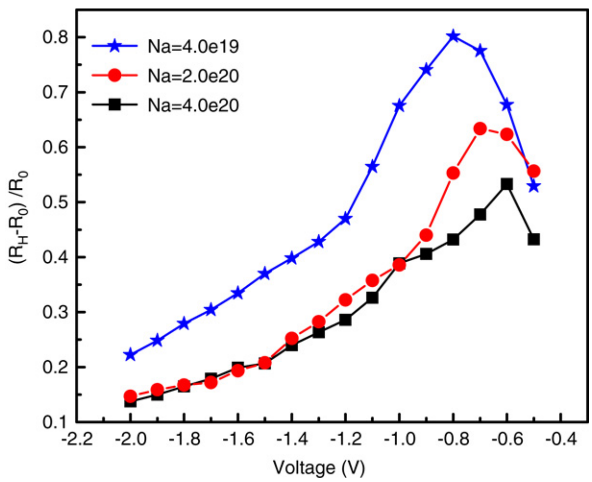

Fig. 3. The dependence of MR value with negative bias at the electron doping concentration being 2.0×10^{20} cm^{-3} for SNTO and various hole concentrations for LSMO in the LSMO/SNTO junction at 255 K with spin polarization of 0.6.

field, electrons in $e_g^1 \uparrow$ band in the homogeneous region of LSMO can only tunnel to $t_{2g} \downarrow$ band which is partly lower than $e_g^2 \uparrow$ band in the space charge region of LSMO. With the increase of negative bias, E_{vp} can equal or even exceed the bottom of $e_g^2 \uparrow$ band. From the energy band structure shown in Fig. 1, it can be seen that the electrons in $e_g^1 \uparrow$ band have the probability tunneling to both $t_{2g} \downarrow$ band and $e_g^2 \uparrow$ band under magnetic field. The spin anti-parallel tunneling causes a decrease of current, while the spin parallel tunneling causes an increase of current. At first, the current tunneling to $t_{2g} \downarrow$ band is larger than that to $e_g^2 \uparrow$ band, so that the value of positive MR increases with bias. When the tunneling current of electrons from $e_g^1 \uparrow$ band to $t_{2g} \downarrow$ band is equal to that to $e_g^2 \uparrow$ band, the positive MR value reaches a maximum. With further increase of negative bias, the current tunneling to $e_g^2 \uparrow$ band increases more rapidly than the increase of that to $t_{2g} \downarrow$, so that the positive MR starts to decrease with bias. Therefore we can conclude that the competition between the current tunneling to the $t_{2g} \downarrow$ band and to $e_g^2 \uparrow$ band leads to the variation of positive MR value under applied negative bias. We can understand that the spin polarization of electron increases with magnetic field, which leads to the increase of MR value with magnetic field. From the comparison of calculated MR and experimental data shown in Fig. 2, we can see a dependence of spin polarization of the system on magnetic field.

Fig. 3 shows the MR value dependence on hole doping concentration of 4.0×10^{19}, 2.0×10^{20}, and 4.0×10^{20} cm^{-3} for LSMO, respectively, and electron doping concentration of 2.0×10^{20} cm^{-3} for SNTO in the LSMO/SNTO junction. It can be seen clearly that higher hole doping concentration leads to a smaller positive MR value. With the increase of hole doping concentration, although the tunneling current increases due to the decrease of the width of the space charge region, the increase of the calculated $J_2(P)$ is smaller than $J(P)$. Therefore, $J(P)$ has more important influence on MR value at a given negative bias than $J_2(P)$ with different hole doping concentration. From the definition of the MR in Eq. (2), the larger tunneling spin current $J(P)$ will lead to a smaller MR value at a given negative bias under magnetic field with different doping concentration. Therefore, the positive MR value should decrease with increasing hole doping concentration. Our calculation result predicts that the magnetoresistance decreases with the increase of doping concentration of p region. We can conclude that lower doping density (like 0.1) causes larger positive MR, although higher doping density (like 0.3) of LSMO causes larger negative MR for LSMO bulk for LSMO/SNTO heterostructures.

In summary, the values of MR with negative bias and hole doping concentration with various spin polarization are obtained by theoretical calculation. The theoretical calculation shows that the variation of MR value with bias agrees well with experimental results. The mechanism of the variation of MR value with negative bias is proposed and verified to be due to the competition between the tunneling rate of electrons in $e_g^1 \uparrow$ band to $t_{2g} \downarrow$ band and that to $e_g^2 \uparrow$ band at the interface region of $La_{0.9}Sr_{0.1}MnO_3$. The mechanism of a lower doping of LSMO causing a larger positive MR of LSMO/SNTO is also revealed. In this letter, a valid model has been presented, by which a complicated CMR problem in oxide heterostructure can be treated, and this model should be applicable for almost all kind of oxide p–n junctions. We believe that the employment of spin current has potential application for designing MR-related devices in perovskite oxides.

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