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Theoretical model of the mechanism study on the positive magnetoresistance in the heterostructure composed of two oxides

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Abstract

A positive colossal magnetoresistance (CMR) has been discovered at low applied magnetic field and in the temperature range from 130 to 290 K in the epitaxial p–n heterostructure fabricated with Sr-doped $LaMnO_3$ and Nb-doped $SrTiO_3$ by laser molecular-beam epitaxy. The mechanism causing the unusual positive CMR is proposed as an interface effect, i.e., creation of the region near the interface with electron filling in the t_{2g} spin-down band in $La_{0.9}Sr_{0.1}MnO_3$ plays a crucial role in spin-dependent carrier transport of the system. Self-consistent calculation has been carried out to obtain the band diagram around the interface of the heterostructure. Other puzzling CMR features, which exhibit values of positive CMR first increase and then decrease with increase of negative bias voltage and temperature, are well explained by the present scenario.
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1. Introduction

The hole-doped manganese oxides of general formula $La_{1-x}B_xMnO_3$ (B = Ca, Sr, Ba, Pb) exhibit very large negative magnetoresistance (MR), called colossal magnetoresistance (CMR) whose value is defined by $MR = (R_H\text{-}R_0)/R_0$ with R_H denoting resistance under applied magnetic field H and R_0 depending the resistance without magnetic field. The understanding of the microscopic physics underlying CMR properties is very important and fundamental. Good results of negative MR have been reported in some magnetic tunnel junctions (MTJ) [1–4]. Recently, positive MR has also been found in some systems [5–8], such as in a multilayer p–n heterostructure of Sr-doped $LaMnO_3$ and Nb-doped $SrTiO_3$ [7]. However, it is very puzzling and even seems incredible that a system with the structure consisting of a nonmagnetic material $SrNb_{0.01}Ti_{0.09}O_3$ (SNTO) and a negative CMR material $La_{0.9}Sr_{0.1}MnO_3$ (LSMO) to give rise to a positive CMR property. The physics origin causing this unusual phenomenon is proposed in this paper as the creation of the space–charge region where t_{2g} spin-down ($t_{2g}\downarrow$) band is partially filled by electrons at the interface of LSMO.

2. Experimental methods

A computer-controlled laser molecular-beam epitaxy (laser MBE) [9] was used to deposit the LSMO/SNTO p–n junctions. The p–n junction was made by depositing LSMO with thickness of 400 nm directly on 1% Nb-doped $SrTiO_3$ (0 0 1), as shown in the inset of Fig. 1. Our XRD θ–2θ scan curve of the LSMO/SNTO p–n heterostructure shows that there exist only LSMO (*0 0 l*) and SNTO (*0 0 l*) peaks without any trace for other diffraction peak from impurity phase or randomly oriented grain, which means that thin films of heterostructure are in single phase with *c*-axis orientation. The cross-sectional high-resolution transmission electron microscopic (HRTEM) image is shown in the inset of Fig. 1.

The measurement was taken in a constant current with a step of 0.01 mA. The I–V behaviors of the LSMO/SNTO p–n junction shown in Fig. 1 were measured in the

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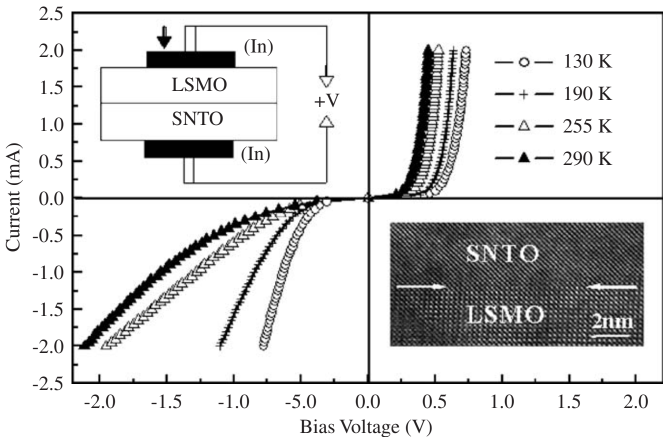

Fig. 1. The I–V curves of $La_{0.9}Sr_{0.1}MnO_3/SrNb_{0.01}Ti_{0.99}O_3$ p–n junction without applied magnetic field at various temperatures. Inset: schematic illustration of the p–n junction and the cross-sectional HRTEM image of the interface of the p–n junction.

temperature range of 130–290 K by a superconducting quantum interference device (SQUID, Quantum Design MPMS 5.5 T). A magnetic field perpendicular to the p–n interface was applied. The character of increased MR with the increased magnetic field at various temperatures is shown in Figs. 2(a)–(d). The magnetic hysteresis loops of LSMO/SNTO heterostructure with the magnetic field perpendicular to the film plane are plotted in Fig. 3 for various temperatures.

3. Theoretical model

To understand the physics inducing the abnormal positive CMR property of this p–n junction structure consisting of a nonmagnetic material (SNTO) and a negative CMR material (LSMO), we present our theoretical calculation for the band diagram of the interface region based on the band structures of LSMO and SNTO. If SNTO is connected with LSMO in an applied magnetic field, the electrons from n type SNTO will diffuse into the adjacent p type LSMO, they even partially fill the t_{2g} spin-down ($t_{2g}\downarrow$) band after filling up the e_g^1spin-up ($e_g^1\uparrow$) band of LSMO near the interface, and then the Schottky barrier is built up around the interface to stop the further diffusion of electrons. Weak Hund's rule coupling [5] (the splitting of $t_{2g}\uparrow$ and $t_{2g}\downarrow$ being smaller than the sum of the crystal field splitting energy between e_g and t_{2g} bands and Jahn–Teller splitting energy between two e_g bands) is proposed here as a hypothesis based on which the existing minority spin carriers [10] in the system is reasonable. As we will see below, creation of the space–charge region with electron filling in the $t_{2g}\downarrow$ band in LSMO is the origin causing the positive CMR in the heterostructure.

In order to show different regions in the structure in an applied magnetic field, we plot in Fig. 4(a) schematically and Fig. 4(b) results from our calculation for the system in equilibrium. In our calculation, Poisson's equation and Boltzmann equation were solved self-consistently for equilibrium carrier densities and for electrostatic potential. Region I in Fig. 4 denotes the LSMO homogeneous region far away from the interface, region II denotes the LSMO space–charge region close to the interface, region III is the SNTO space–charge region close to the interface, and region IV is the SNTO homogeneous region far away from the interface. In Fig. 4, E_F denotes the Fermi level in the system, E_g denotes the band gap between $t_{2g}\downarrow$ and $e_g^1\uparrow$, and ΔE is the energy deference between $e_g^1\uparrow$ band edge and $t_{2g}\downarrow$ band edge in LSMO. E_g is smaller than the band gap between the two bands of $e_g^1\uparrow$ and $e_g^2\uparrow$ ($\approx$ 1.0 eV) due to the weak Hund's rule coupling [5]. The value of ΔE is $\sim$ 0.2 eV. The MR across such a p–n junction of the magnetic and a nonmagnetic compound depends on the relative spin orientation of electrons around the Fermi level in each region where the spin polarised carriers pass through.

4. Results and discussion

Now we focus on the positive CMR dependence on the applied negative bias V under which the Fermi level of region I is raised with respect to that of region IV. We can approximately present (causing the positive MR) the part of current (decreasing) ΔI_+ with the magnetic field H and (causing the negative MR) the part of current (increasing) ΔI_- with H

$$\Delta I_+ = I_+^0 - I_+^H \propto \mathrm{DOS_I}(E_{e^1\uparrow}) \times \mathrm{DOS_{II}}(E_{t\downarrow}), \tag{1}$$

$$\Delta I_- = I_-^H - I_-^0 \propto \mathrm{DOS_I}(E_{e^1\uparrow}) \times \mathrm{DOS_{II}}(E_{e^2\uparrow}), \tag{2}$$

where $\mathrm{DOS_I}(E_{e^1\uparrow})$ denotes the DOS at the electron filling level of e_g^1 band in region I, $\mathrm{DOS_{II}}(E_{e^2\uparrow})$ denotes the DOS of carries involved in the current in e_g^2 band in region II, and $\mathrm{DOS_{II}}(E_{t\downarrow})$ denotes the DOS of carries involved in the current in $t_{2g}\downarrow$ band in region II under the bias V. Only if $\Delta I_+ > \Delta I_-$, the system can show a positive MR property. From above equations, it can be clearly seen that the electron filling in $t_{2g}\downarrow$ band in region II and the tunnelling process are the origin causing the positive MR. Furthermore, competition between two sources of currents (Eqs. (1) and (2)) plays a crucial role in MR evolution with various measuring conditions of the system. At the bias $|V|$ much smaller than E_g, electrons in the region I hardly tunnel the barrier E_g to flow to the region II, thus almost no current flows in the system. This corresponds to what we observed at small negative bias voltage in Fig. 2. With $|V|$ being larger than a certain value, the Fermi level of region I shifted up enough to reach the bottom of e_g^2 band of region II, tunnelling current occurs, so that both the majority channel of e_g^2 and the minority channel of $t_{2g}\downarrow$ in region starts to be available for transport. The scattering of spin–up electrons in e_g^1 of region I with spin-down electrons in $t_{2g}\downarrow$ of II increases with applied magnetic field, which causes positive MR in the system. The increasing of reverse bias voltage increases the Fermi level in region I, and thus makes more and more electrons filling of e_g^2 in region II and being involved in the transport, which causes the MR value

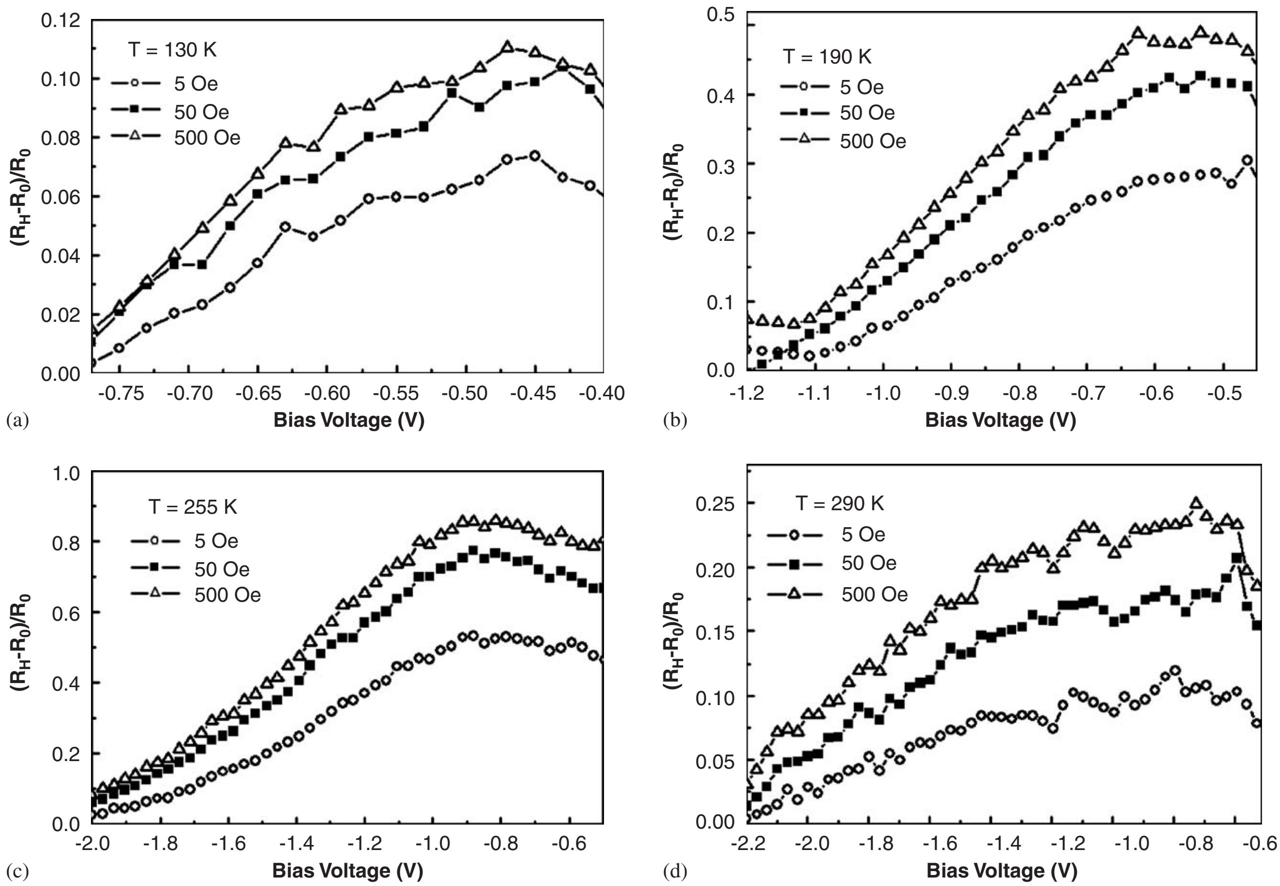

Fig. 2. The variation of MR values of of the system with negative bias voltage under different applied magnetic fields at temperatures 130 K (a), 190 K (b), 255 K (c), and 290 K (d).

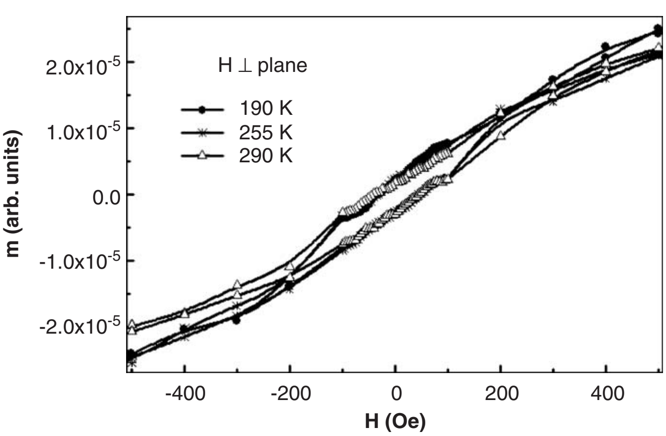

Fig. 3. The magnetic hysteresis loops of LSMO/SNTO heterostructure with magnetic field perpendicular to the film plane for various temperature.

to starts decrease with increasing $|V|$. This behavior of MR depending on the bias voltage agrees well with the phenomenon shown in Fig. 2.

The temperature dependence of positive MR in Fig. 2 can also be understood by this scenario as in the following. With increasing temperature, electron filling of the $t_{2g}\downarrow$ band in

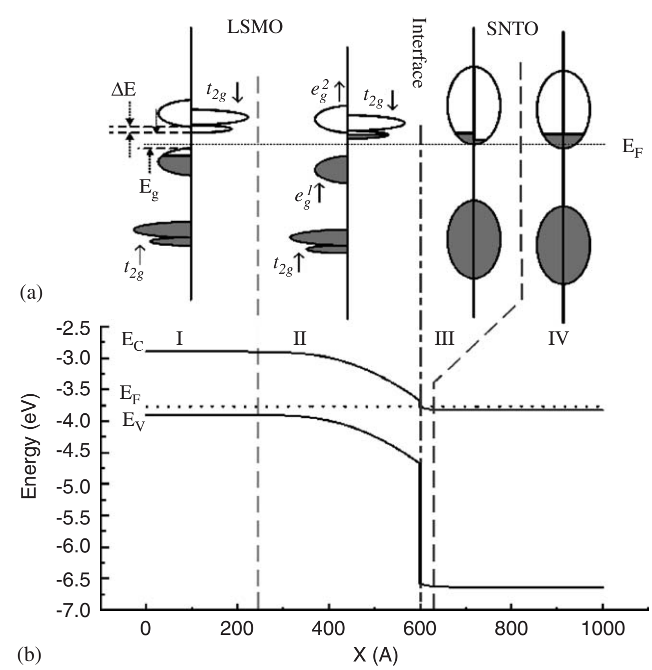

Fig. 4. The schematic DOS of the p–n junction (a), and the corresponding band diagram for each region (b).

region II increases, so also is the positive MR in the system, which corresponds to MR evolution from 130 to 225 K. If we further increased the temperature, electrons start to fill e_g^2 in region II and that causes MR value to decrease, which corresponds to the MR variation from 225 to 290 K.

In summary, positive MR properties of LSMO/SNTO p–n junction have been reported and the origin of the puzzling phenomena has been proposed as the electron filling in the spin-down band in the space-charge region of LSMO close to the interface and the tunnelling process in different region of LSMO. Meanwhile, spin-up (e_g^2) carriers of region II in transport play a crucial role in the MR evolution at various measuring conditions.

Acknowledgements

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