A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

OFFPRINT

A theoretical study on the transport property of the $La_{0.7}Sr_{0.3}MnO_3$/Si p-n heterojunction

JIE QIU, KUI-JUAN JIN, PENG HAN, HUI-BIN LU, CHUN-LIAN HU, BAO-PING WANG and GUO-ZHEN YANG

EPL, **79** (2007) 57004

TAKE A LOOK AT THE NEW EPL

Europhysics Letters (EPL) has a new online home at
www.epljournal.org

Take a look for the latest journal news and information on:

- reading the latest articles, free!
- receiving free e-mail alerts
- submitting your work to EPL

www.epljournal.org

A Letters Journal Exploring the Frontiers of Physics

September 2007

EPL, **79** (2007) 57004 www.epljournal.org
doi: 10.1209/0295-5075/79/57004

A theoretical study on the transport property of the $La_{0.7}Sr_{0.3}MnO_3$/Si p-n heterojunction

Jie Qiu, Kui-juan Jin[(a)], Peng Han, Hui-bin Lu, Chun-lian Hu, Bao-ping Wang and Guo-zhen Yang

Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academic of Sciences - Beijing 100080, China

received 8 June 2007; accepted in final form 6 July 2007
published online 30 July 2007

PACS 73.40.Lq – Other semiconductor-to-semiconductor contacts, *p-n* junctions, and heterojunctions
PACS 72.20.Dp – General theory, scattering mechanisms
PACS 75.47.Lx – Manganites

Abstract – The transport property of the $La_{0.7}Sr_{03}MnO_3$/Si heterostructure was investigated theoretically by applying the drift-diffusion model to the present system. A simple scenario of the semiconductor band and electric field at the interface region of the heterostructure with various bias voltages are presented. The good agreement between the self-consistent calculated results and the experimental data indicates that the proposed band picture is valid for the interpretation of the transport property of the *p-n* heterojunctions made of $La_{0.7}Sr_{0.3}MnO_3$ and Si regardless of the complexity of the interface structures and multi-couplings among charge, spin, lattice and orbital of manganites.

Introduction. – Perovskite manganese oxides $La_{l-x}A_xMnO_3$ (where A stands for divalent ions like Sr, Ca, Ba) well known for their outstanding colossal-magnetoresistance effect (CMR) have exhibited various physical contexts due to multiple couplings among charge, spin and orbital degrees of freedom [1]. Various models have been established to explain the transport properties of $La_{l-x}A_xMnO_3$, such as double exchange theory [2], phase separation mechanism [3] and electron-phonon coupling effect [4]. Recently, great efforts have been devoted to the fabrication of oxide semiconductor devices based on the perovskite oxide films whose properties could be controlled by magnetic field, electric field and light irradiation. Many interesting phenomena like positive colossal magnetoresistance from interface effect [5], and photovoltaic effects [6] have been reported. Integrating the perovskite-type transition metal oxides with the silicon-based semiconductor technology would introduce the possibility for a multifunctional microelectronic device. Lord K. *et al.* investigated the rectifying behaviors of the $La_{0.7}Sr_{0.3}MnO_3$/Si (LSMO/Si) *p-n* junctions [7]. We also reported the transport property of the LSMO/Si heterojunction [6]. However, no corresponding theoretical work has been reported so far. Generally speaking, the e_g electrons in perovskite manganese oxides were thought to be localized in the perovskite manganese oxides because of the strong Hund's rule coupling between the e_g electrons and t_{2g} electrons, and the e_g electrons should be correlated by the dynamic Jahn-Teller distortion and the strong Coulomb repulsion [8]. Therefore there is a general speculation that the band theory for traditional semiconductor device could not be applied to perovskite-type transition metal oxides. Chambers *et al.* measured the valence and conduction band offsets at $SrTiO_3$/Si (001) interface, and revealed the characteristics of the band structure of $SrTiO_3$/Si [9]. Our early theoretical work also confirmed that the band picture can interpret the transport property of the $SrTiO_3$ *p-n* homojunction [10]. In order to further investigate the application of band scenario to the transport property of *p-n* heterostructures based on perovskite manganese oxides, we present a self-consistent calculation to theoretically explain the transport property of the LSMO/Si heterojunction by solving the current continuity equations and Poisson equation on the basis of the drift-diffusion theory. The good agreement between our numerically calculated results and the experimental data indicates that the band picture can still be a good approach to describe the transport property of *p-n* heterojunctions consisting of perovskite oxides with multiple couplings among charge, spin and orbital degrees of freedom.

[(a)] E-mail: kjjin@aphy.iphy.ac.cn

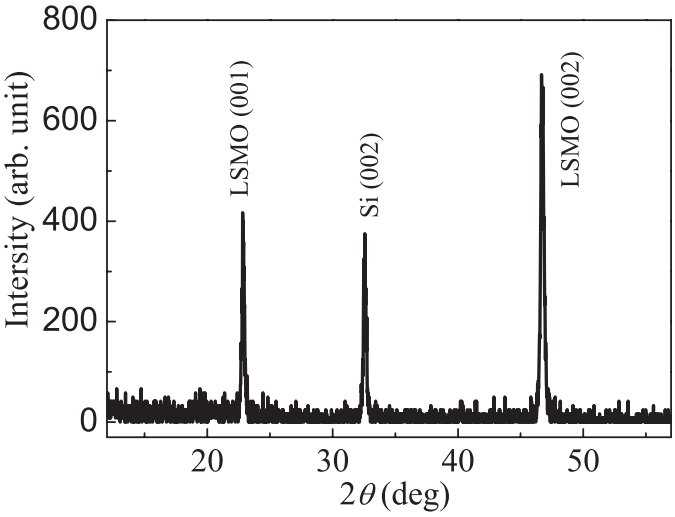

Fig. 1: XRD pattern of a 500 nm thick LSMO film on a Si (00l) substrate we fabricated.

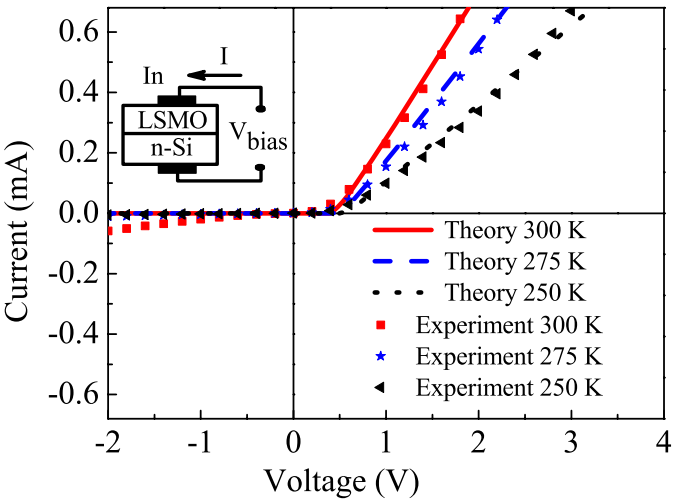

Fig. 2: The experimental and theoretical results of I-V curves in the heterostructure of LSMO/Si over the temperature range of 250–300 K.

Experiment and numerical calculation. – The LSMO/Si heterojunctions were obtained by depositing 500 nm thick LSMO films (work function of 4.96 eV [11] and band gap of 1.0 eV [12]) on the n-Si substrate (work function of 4.25 eV and band gap of 1.12 eV [13]) by laser molecular-beam epitaxy (laser-MBE). The fabrication process of LSMO/Si heterojunctions was described in detail elsewhere [6]. θ-2θ X-ray diffraction was carried out to examine the crystalline quality of the LSMO thin film on a Si (00l) substrate, the results of which are shown in fig. 1. To measure the transport characteristics of the LSMO/Si heterojunction, indium (In) electrodes ($2 \times 2\,\mathrm{mm}^2$) were symmetrically attached the surface of the LSMO film and of the Si wafer as shown in the inset of fig. 2. The current-voltage characteristics of the LSMO/Si heterojunction were measured with a pulse-modulated voltage source.

To gain the insight into the nature of the transport property at the interface region of the heterostructure, we apply the current continuity equations and Poisson equation on the basis of the drift-diffusion theory for calculating the band structure and the electric field of the p-n heterojunction under various bias voltages [14]. The Poisson equation, for a one-dimensional analysis, can be written as follows:

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = -(q/\varepsilon)(p(x) - n(x) + N), \tag{1}$$

where $\psi(x)$ is the electric potential, q is the elementary charge, ε is the permittivity of a semiconductor which is taken as 10 for LSMO [15] and 11.9 for Si [13], $p(x)$ is the carrier hole concentration, $n(x)$ is the carrier electron concentration and the parameter N is the net impurity concentration which is taken as $10^{20}\,\mathrm{cm}^{-3}$ for LSMO from our Hall measurement and $10^{16}\,\mathrm{cm}^{-3}$ for Si [13]. For the one-dimensional case under a steady state, the continuity equations is

$$\begin{aligned} q\,(G_n(x) - U_n(x)) + \frac{\mathrm{d}J_n}{\mathrm{d}x} &= 0, \\ q\,(G_p(x) - U_p(x)) - \frac{\mathrm{d}J_p}{\mathrm{d}x} &= 0, \end{aligned} \tag{2}$$

where $G_n(x)$ and $G_p(x)$ are the electron and hole generation rate, respectively, $U_n(x)$ is the electron recombination rate in p-type semiconductor, and $U_p(x)$ is the hole recombination rate in n-type semiconductor. J_n and J_p are the electron current density and the hole current density, respectively, which can be described as follows:

$$\begin{aligned} J_n &= -q\mu_n \left(n(x)\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} - (kT/q)\frac{\mathrm{d}n(x)}{\mathrm{d}x} \right), \\ J_p &= -q\mu_p \left(p(x)\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} + (kT/q)\frac{\mathrm{d}p(x)}{\mathrm{d}x} \right), \end{aligned} \tag{3}$$

where μ_p is the hole mobility which is taken as $500\,\mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$ for Si [13] and $1.8\,\mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$ for LSMO from our Hall measurement, μ_n is the electron mobility which is taken as $10\,\mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$ for LSMO and $1350\,\mathrm{cm}^2/\mathrm{V}\cdot\mathrm{s}$ for Si [13], and the parameters k and T are Boltzmann constant and the ambient temperature, respectively. The electron effective mass is taken as $1.06\,m_\mathrm{e}$, and the hole effective mass is taken as $0.59\,m_\mathrm{e}$ for Si [13]. The effective mass for LSMO is taken as $4\,m_\mathrm{e}$ [15]. The parameter m_e is the free electron rest mass.

Using boundary condition of various bias voltages and self-consistently solving Poisson's equation (1) and the current-continuity equation (2) by using Newton's iteration method and the uncoupled method, we obtained the I-V characteristics. The band structure and the electric field in the space charge region of the LSMO/Si heterojunction under forward, reverse, and zero bias, respectively, can also be obtained.

Results and discussion. – Figure 1 exhibits a typical XRD pattern of a 500 nm thick LSMO film growing directly on the Si (00l) substrate. Except for (00l) diffraction peaks of the Si substrate and the LSMO film, no other diffraction peaks from impurity phases or randomly oriented grains were found, which indicates that the LSMO film was grown exclusively along the (00l) direction. This result can be understood as follows. The in-plane lattice parameter is about 5.43 Å for Si, and about 3.86 Å for LSMO. With the LSMO unit cell rotating 45° around the Si surface normal [100] axis, the lattice mismatch between LSMO and Si is about 0.55%. The small lattice mismatch allows a nearly epitaxial growth of LSMO on Si substrate.

Figure 2 presents the experimental and theoretical results of I-V curves of the LSMO/Si heterostructure over the temperature range of 250–300 K. The solid, dashed, dotted lines represent the theoretical current-voltage characteristics at the temperature of 300 K, 275 K and 250 K, respectively, and the experimental data obtained at 300 K, 275 K and 250 K are denoted by solid squares, solid stars, and solid triangles, respectively. The experimental data clearly present asymmetric I-V curves of the LSMO/Si heterojunctions. Considering the effect of contact resistance and substrate resistance on the transport property of the LSMO/Si heterostructure, we introduced series resistances into the calculation of I-V characteristics. The series resistance was taken as 2 kΩ, 2.5 kΩ and 3.8 kΩ at 250 K, 275 K, and 300 K, respectively. The theoretical calculation results show the currents increased rapidly with the increasing forward-bias voltages, which was in good agreement with the experimental data in the forward-bias case. Therefore it is reasonable that we apply the drift-diffusion theory for calculating the band structure and the electric field of the p-n heterojunction under forward bias voltages. Moreover, like other experimental studies [6,7], it is feasible to disregard the effect of an unavoidable ultrathin layer of SiO_2 between Si substrate and epitaxial LSMO film on the transport properties of LSMO/Si heterojunction in this paper. The diversion between the calculation results and experimental results in the reverse-bias case is mainly due to the neglect of the leakage current and the tunneling current in the calculation.

Figure 3 and 4 show the calculated energy-band diagram and the electric field of the space charge region, respectively, of the LSMO/Si heterojunction under forward, reverse and zero bias. The solid, dotted and dashed lines represent the energy-band features and the electric field of the LSMO/Si heterojunctions under applied biases of 0 V, 0.4 V, and −0.4 V, respectively. The vertical short dotted line denotes the position of the interface of the LSMO/Si heterojunction. Figure 3 shows that the potential barrier of the LSMO/Si heterojunction decreases under a forward bias, and increases under a reverse bias. We can also see that the space charge region mainly located in the n-Si region, which is caused by the much smaller carrier

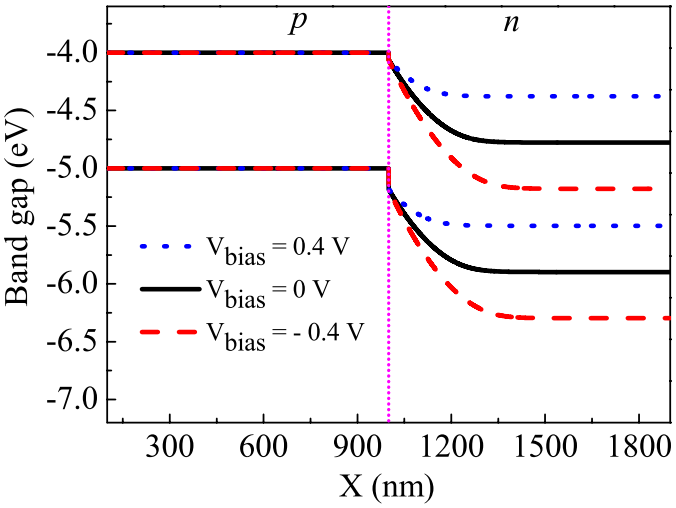

Fig. 3: The calculated energy-band diagrams of the LSMO/Si heterojunction under applied bias voltages of 0.4 V, −0.4 V, and 0 V.

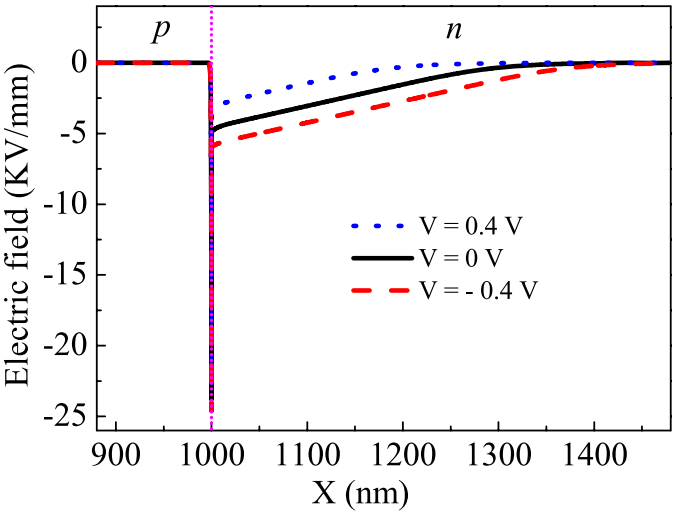

Fig. 4: Electric fields of the space charge region of the LSMO/Si heterojunction obtained by solving eqs. (1) and (2) under applied bias voltages of 0 V, 0.4 V, and −0.4 V. The vertical short dotted line denotes the interface of the LSMO/Si heterojunction.

concentration of Si than that of LSMO. Figure 4 shows the values of the electric field in the space charge field under a negative bias of −0.4 V were larger than those without bias. On the contrary, the values of the electric field in the space charge field under a positive bias of 0.4 V were smaller than those without bias. The maximum magnitude of the electric field under various biases exits at the interface of the LSMO/Si heterostructure.

Conclusions. – In summary, the transport characteristics of the LSMO/Si p-n heterojunction were investigated theoretically by numerically solving one-dimensional steady-state carrier-transport equations based on the drift-diffusion model. The band structure

and electric field at the interface region were obtained at various bias voltages, which showed some insight into the nature of the transport property of the complicated system. The good agreement between the calculated results and the measured data over the temperature range of 250–300 K indicates that the energy band scenario can still be a good approach to describe the transport property of the LSMO/Si heterostructure in which the perovskite oxide is with multiple couplings among charge, spin and orbital degrees of freedom.

* * *

The authors would like to thank the support from National Natural Science Foundation of China and National Basic Research Program of China No. 2007CB307005.

REFERENCES

[1] Jin S. *et al.*, *Science*, **264** (1994) 413; Helmolt R. V. *et al.*, *Phys. Rev. Lett.*, **71** (1993) 2331; Zhang J. D. *et al.*, *Phys. Rev. Lett.*, **86** (2001) 3823.

[2] Zener C., *Phys. Rev.*, **82** (1951) 403; Millis A. J., *Nature*, **392** (1998) 147.

[3] Goodenough J. B. and Zhou J. S., *Nature*, **386** (1997) 229; Fäth M. *et al.*, *Science*, **285** (1999) 1540; Zhou Q. L. *et al.*, *Phys. Rev. B*, **72** (2005) 224439; *Appl. Phys. Lett.*, **87** (2005) 172510.

[4] Millis A. J., *Phys. Rev. B*, **53** (1996) 8434; Millis A. J. *et al.*, *Phys. Rev. Lett.*, **74** (1995) 5144; Dai P. *et al.*, *Phys. Rev. B*, **54** (1996) R3694.

[5] Lu H. B. *et al.*, *Appl. Phys. Lett.*, **82** (2005) 032502; Jin K. J. *et al.*, *Phys. Rev. B*, **71** (2005) 184428.

[6] Lu H. B. *et al.*, *Appl. Phys. Lett.*, **86** (2005) 241915.

[7] Lord K. *et al.*, *Appl. Phys. Lett.*, **89** (2006) 052116.

[8] Anderson P. W. and Hasegawa H., *Phys. Rev.*, **100** (1955) 675; Tanaka H., Zhang J. and Kawai T., *Phys. Rev. Lett.*, **88** (2002) 027204; Millis A. J., Shraiman B. I. and Mueller R., *Phys. Rev. Lett.*, **77** (1996) 175.

[9] Chambers S. A. *et al.*, *Appl. Phys. Lett.*, **77** (2000) 1662.

[10] Zhou Q. L. *et al.*, *Europhys. Lett.*, **71** (2005) 283.

[11] Kudo T. *et al.*, *Jpn. J. Phys.*, **37** (1998) 999.

[12] Zhao K. *et al.*, *Appl. Phys. Lett.*, **88** (2006) 141914.

[13] Liu E. K., Zhu S. B. and Luo S. J., *Physics of Semiconductor* (Academic, Beijing) 2003.

[14] Sze S. M., *Physics of Semiconductor Devices* (Wiley, New York) 1981.

[15] Wang L. M. *et al.*, *J. Appl. Phys.*, **95** (2004) 4928.