ISSN: 0256-307X

中国物理快报

Chinese Physics Letters

Volume 26 Number 5 May 2009

A Series Journal of the Chinese Physical Society
Distributed by IOP Publishing

Online: http://www.iop.org/journals/cpl
http://cpl.iphy.ac.cn

CHINESE PHYSICAL SOCIETY

CHIN. PHYS. LETT. Vol. 26, No. 5 (2009) 057301

Acceptor Concentration Effects on Photovoltaic Response in the $La_{1-x}Sr_xMnO_3/SrNb_yTi_{1-y}O_3$ Heterojunction *

LIAO Leng(廖棱), JIN Kui-Juan(金奎娟)**, HAN Peng(韩鹏), ZHANG Li-Li(张莉莉), LÜ Hui-Bin(吕惠宾), GE Chen(葛琛)

Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academic of Sciences, Beijing 100190

(Received 16 October 2008)

Photovoltaic response in the heterojunction of $La_{1-x}Sr_xMnO_3/SrNb_yTi_{1-y}O_3$ (LSMO/SNTO) is analyzed theoretically based on the drift-diffusion model. It is found that the decrease of acceptor concentration in the $La_{1-x}Sr_xMnO_3$ layer of heterojunction can increase the peak value of photovoltaic signal and the speed of photovoltaic response, whereas the changing of donor concentration in the $SrNb_yTi_{1-y}O_3$ layer has no such evident effect. Furthermore, the result also indicates that the modulation of Sr doping in $La_{1-x}Sr_xMnO_3$ is an effective method to accommodate the sensitivity and the speed of photovoltaic response for LSMO/SNTO photoelectric devices.

PACS: 73.40.Lq, 72.40.+w, 78.20.Bh

On account of the strong electron correlation, pervoskite oxides exhibit a rich variety of properties. Since the colossal magnetoresistance (CMR)[1] was found in the manganite oxide, a great deal of attention has been paid to manganite materials. $La_{1-x}Sr_xMnO_3$(LSMO) is a typical manganite material that is valuable in both fundamental research and real applications. In LSMO, the complex interplay between magnetic and electronic properties relies strongly on the doping concentration,[2] which can be achieved by chemical substitution of constituent elements. Beyond the usual chemical method, the carrier concentration near the interface of the heterojunction can be controlled by applying external field, such as electric field and light, which can induce many interesting phenomena.[3,4] Recently, many unusual photoelectric effects have been found in the heterojunction of $La_{1-x}Sr_xMnO_3/SrNb_yTi_{1-y}O_3$ (LSMO/SNTO). Katsu *et al.* found the photocarrier injection effect in ferromagnetic-$La_{1-x}Sr_xMnO_3$/photoactive-$SrTiO_3$ heterojunction and achieved dynamic light control of magnetic and electric transport properties of $La_{1-x}Sr_xMnO_3$.[5] In our previous work, we observed unusual lateral photoelectric effect in the $La_{0.9}Sr_{0.1}MnO_3/SrNb_{0.01}Ti_{0.99}O_3$ heterojunctions and explained it by the Dember effect.[6] Therefore, the theoretical study on the photoelectric effect in LSMO/SNTO heterojunction is highly desired.

In this Letter, we give a theoretical description of photovoltaic effect in the LSMO/SNTO heterojunction by introducing a time-dependent drift-diffusion model, consisting of Poisson equation and time-dependent electron and hole continuity equations. We solve these equations self-consistently by numerical methods: finite difference, Newton algorithm and classical implicit scheme. The time-dependent drift-diffusion model is a development of the stable drift-diffusion model. In the previous works of our group, the stable drift-diffusion model has been successfully exploited to study the transport properties in perovskite heterojunctions.[7] In this study, we present the calculated results. The reduction of acceptor concentration in the LSMO layer can increase both sensitivity and speed of photovoltaic response in the LSMO/SNTO heterojunction, but the changing of donor concentration in the SNTO layer does not have such effects. This result is explained by the great difference between dielectric properties and doping concentrations in LSMO and SNTO, and their different effects on the junction-capacitance of LSMO/SNTO heterojunction.

The basic equations of time-dependent drift-diffusion model are the Poisson equation and the electron and hole continuity equations,[8] i.e.

$$\frac{\partial^2\phi(x,t)}{\partial x^2} = h^2\frac{e}{\varepsilon}(n(x,t) - p(x,t) - N), \quad (1)$$

$$\frac{\partial p(x,t)}{\partial t} = -\frac{1}{e}\frac{dj_p(x,t)}{dx} + G(x,t) - R(x,t), \quad (2)$$

$$\frac{\partial n(x,t)}{\partial x} = \frac{1}{e}\frac{dj_n(x,t)}{dx} + G(x,t) - R(x,t), \quad (3)$$

$$j_p(x,t) = -e\mu_p p(x,t)\frac{\partial\phi(x,t)}{\partial x} - kT\mu_p\frac{\partial p(x,t)}{\partial x}, \quad (4)$$

$$j_n(x,t) = -e\mu_n n(x,t)\frac{\partial\phi(x,t)}{\partial x} + kT\mu_n\frac{\partial n(x,t)}{\partial x}. \quad (5)$$

The evolutions of electrostatic potential $\Psi(x,t)$, electron concentration $n(x,t)$ and hole concentration $p(x,t)$ in homogeneous region of heterojunction are

*Supported by the National Natural Science Foundation of China and the National Basic Research Program of China

**To whom correspondence should be addressed. Email: kjjin@aphy.iphy.ac.cn

all determined by the above five equations, in which $j_n(x,t)$ and $j_p(x,t)$ denote the electron and hole current densities, respectively; e, ε and N denote the electron charge, dielectric permittivity and net ionized impurity concentrations, respectively; μ_n and μ_p are the electron and hole mobilities; k and T represent Boltzmann constant and temperature taken as room temperature in this work, respectively. The electron-hole pair generation rate $G(x,t)$ can be expressed as $G(x,t) = I_0(t)\alpha\beta\exp(-\alpha(x)x)$ with $I_0(t)$ denoting the density of incident photon flux, α the absorption coefficient, and β the quantum efficiency. The recombination rate $R(x,t)$ is adopted as the Shockley-Read-Hall (SRH) model.[9] Moreover, the electron and hole movement across the interface of heterojunction is taken into account by the Richardson thermionic emission current model,[10] which has been generally applied on semiconductor heterostructures. The initial values of $\Psi(x,t)$, $n(x,t)$ and $p(x,t)$ needed for solving Eqs. (1)–(5) are obtained by solving the nonlinear Poisson equations.[8] The necessary material parameters are all listed in Table 1.

Table 1. Necessary material parameters (Refs. [4,7,13]) used in the calculation.

	$La_{0.9}Sr_{0.1}MnO_3$	$SrNb_{0.01}Ti_{0.99}O_3$
Dielectric permittivity (ε_0)	10	150
Electron mobility ($cm^2/(V{\cdot}s)$)	10	33
Hole mobility ($cm^2/(V{\cdot}s)$)	1.8	6
Band gap (eV)	1.0	2.8
Affinity energy (eV)	3.9	4.0
Absorption parameters (cm^{-1})	1.2×10^5	1.5×10^5
Quantum efficiency	0.03	0.03

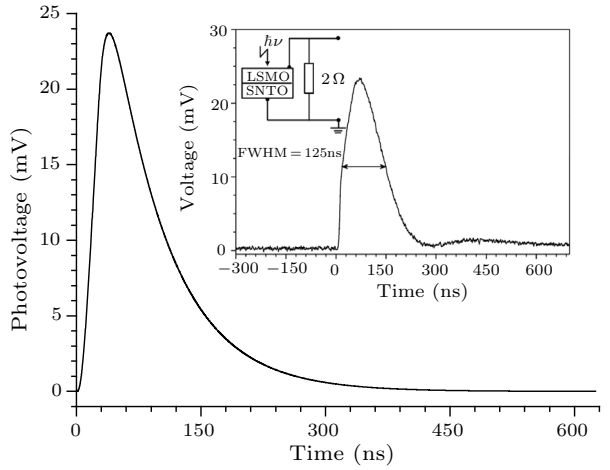

Fig. 1. Calculated time-dependent photovoltage evolution in $La_{0.9}Sr_{0.1}MnO_3/SrNb_{0.01}Ti_{0.99}O_3$ heterojunction. Insert: the corresponding experimental data taken from Ref. [11].

Figure 1 exhibits the good agreement between the calculated and experimental results[11] for photovoltaic effects in $La_{0.9}Sr_{0.1}MnO_3/SrNb_{0.01}Ti_{0.99}O_3$ heterojunction. It is irradiated by a 308-nm and 0.5-mJ·mm^{-2} laser pulse with 25 ns duration and connected by a 2 Ω resistance. From the Hall measurement,[11] the hole concentration in the $La_{0.9}Sr_{0.1}MnO_3$ layer is $1.19 \times 10^{18}\,cm^{-3}$ and the electron concentration in $SrNb_{0.01}Ti_{0.99}O_3$ is $1.63 \times 10^{20}\,cm^{-3}$.

When the LSMO/SNTO heterojunction is illuminated by laser with the photon energy greater than the band gaps of LSMO and SNTO, the electrons in the valence band can be excited into the conduction band, and the corresponding holes are left in the valence band, as shown in Fig. 2. When these photo-created electrons and holes diffuse into the space-charge region, the photo-created ones are separated by the built-in field. Consequently, these photo-created holes and electrons accumulate in p-LSMO and n-SNTO regions, respectively. Thus the Fermi level in n-region is elevated relative to that in p-regions and the photovoltage is created. This process of photovoltage increasing can be considered as charging junction-capacitance of LSMO/SNTO heterojunction. Correspondingly, the process of photovoltage decaying can be regarded as discharging junction-capacitance. Without irradiation, the photo-created carriers can leak out the heterojunction through the parallel resistance and the charge in junction-capacitance decreases. Therefore, the charging and discharging processes of resistance-capacitance (RC) circuit can be used to describe the whole process of photovoltaic effect in LSMO/SNTO heterojunction.

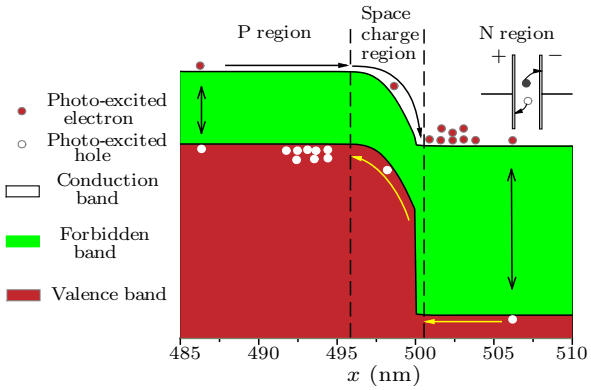

Fig. 2. Movement of photo-created electrons and holes in LSMO/SNTO heterojunction. It is approximated to a process of charging capacitance.

The decay of voltage in an RC circuit is expressed as an exponential decay:

$$V(t) = V(0)\exp(-t/RC), \tag{6}$$

where t, R and C denote time, resistance and capacitance, respectively, $V(t)$ denotes potential between two capacitance's electrodes, respectively. From Eq. (6) and the above analysis for photovoltaic effect, we can see that the junction-capacitance of heterojunction is a critical factor for the time-dependent photovoltage evolution process, and the decay time of photovoltage decreases with the decrease of C.

For the abrupt heterojunction, the junction capac-

itance $C_{\rm jun}$ is approximately given by[12]

$$C_{\rm jun} = \frac{dQ}{dV} = S \cdot \sqrt{\frac{q\varepsilon_n\varepsilon_p N_A N_D}{2(N_D\varepsilon_n + N_A\varepsilon_p)(V_D - V)}}, \quad (7)$$

where S denotes the cross-section area of heterojunction, N_A and N_D denote the acceptor and donor concentration in p- and n-regions, respectively, ε_p and ε_n denote the dielectric permittivity in p- and n-regions, and V_D and V denotes built-in potential barrier and applied bias, respectively. According to Eq. (6), the speed of voltage-decay depends on the junction-capacitance, which is the function of doping concentrations. Thus the doping density has a strong effect on the speed of photovoltaic response in LSMO/SNTO heterojunction. For investigating the effect of doping concentrations on the speed of voltage-decay, we rigorously calculate the photovoltage evolution in LSMO/SNTO heterojunction with various doping densities. In the calculation, we assume that the LSMO/SNTO heterojunction is connected to a 2 Ω resistance and illuminated with a 308-nm and 0.5-mJ·mm^{-2} laser pulse with duration 25 ns. These laser parameters are all identical to those in Ref. [11].

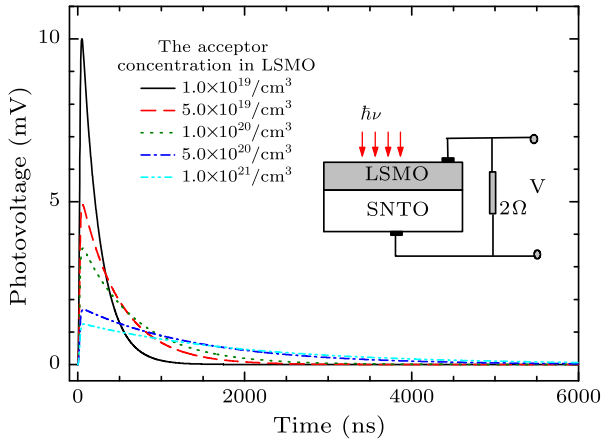

Fig. 3. Calculated time-dependent photovoltage evolution in LSMO/SNTO heterojunctions with different acceptor concentrations in the LSMO layer with doping concentration $1.0 \times 10^{21}/\mathrm{cm}^3$ in the SNTO layer.

Figure 3 shows the time-dependent photovoltage evolution in LSMO/SNTO heterojunction with different acceptor concentration in the LSMO layer and donor concentration keeping $1.0 \times 10^{21}\,\mathrm{cm}^{-3}$ in the SNTO layer. With the increasing acceptor concentration in LSMO, the peak of photovoltage decreases and full width at half maximum (FWHM) is widened. Thus, with the increase of acceptor concentration, the sensitivity of photovoltaic response in LSMO/SNTO is increased and the speed is decreased. Furthermore, Fig. 4 shows another case of time-dependent photovoltage evolutions with variation of donor concentration in the SNTO layer and acceptor concentration in the LSMO layer keeping $1.0 \times 10^{20}\,\mathrm{cm}^{-3}$. As shown in this figure, the changing of donor concentration in the SNTO layer has no evident effect on the photovoltage evolution in LSMO/SNTO heterojunction.

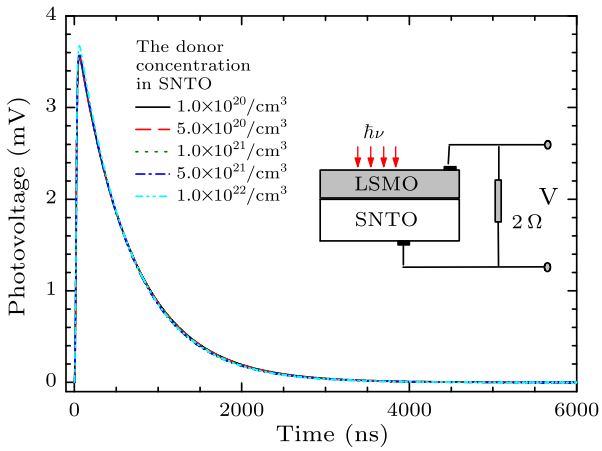

Fig. 4. Calculated time-dependent photovoltage evolution in LSMO/SNTO heterojunctions with different donor concentrations in the SNTO layer with doping concentration $1.0 \times 10^{20}/\mathrm{cm}^3$ in the LSMO layer.

The difference between these effects on the photovoltage evolution in LSMO/SNTO heterojunction is caused by the large difference between dielectric properties and doping concentration in LSMO and SNTO. The dielectric permittivity ε_n of SNTO is much larger than that in LSMO (ε_p) as shown in Table 1. Moreover, the doping concentration in SNTO, N_D, is always larger than that in LSMO (N_A) too. Thus, for LSMO/SNTO heterojunction, Eq. (5) can be reduced to

$$C_{\rm jun} = \frac{dQ}{dV} = S\sqrt{\frac{q\varepsilon_n\varepsilon_p N_A N_D}{2(N_D\varepsilon_n + N_A\varepsilon_p)(V_D - V)}}$$
$$\approx S\sqrt{\frac{q\varepsilon_p N_A}{2(V_D - V)}}, \ \text{for } \varepsilon_n N_D \gg \varepsilon_p N_A. \quad (8)$$

According to Eq. (8) the change of N_A in the LSMO layer has a crucial effect on the junction-capacitance of LSMO/SNTO heterojunction. The junction-capacitance decreases with the decreasing N_A. Furthermore, due to Eq. (6), the decrease of N_A can induce the increase of photovoltage decaying speed. Moreover, when the junction-capacitance decreases, the photovoltage increases in consideration of $V = Q/C$. Thus it explains the results shown in Fig. 3. The peak value and decaying speed of photovoltage increases with the decrease of acceptor concentration in the LSMO layer. In other cases, Eq. (8) also indicates that the shift of junction-capacitance leaded by the change of donor concentration N_D in SNTO can be omitted. Thus, based on the above analysis, the change of N_D would have no evident effect on the photovoltage evolution as shown in Fig. 4.

In summary, the photovoltaic responses in LSMO/SNTO heterojunctions with various doping concentration are theoretically studied on the basis of

drift-diffusion models. Our results reveal that the decrease of Sr doping concentration in the p-type LSMO layer can increase the sensitivity and speed of photovoltaic response in LSMO/SNTO heterojunction. However, the changing of Nb doping concentration in the SNTO layer has no such effect. These results indicate that the modulation of acceptor concentration in LSMO is more effective than that of donor concentration in $SrNb_yTi_{1-y}O_3$ for accommodating the sensitivity and the speed of photovoltaic response in the LSMO/SNTO photo-electronic devices.

References

[1] Jin S, Tiefel T H, McCormack M, Fastnacht R A, Ramesh R and Chen L H 1994 *Science* **15** 264

[2] Urushibara A, Moritomo Y, Arima T, Asamitsu A, Kido G and Tokura Y 1995 *Phys. Rev.* B **51** 14103

[3] Tanaka H, Zhang J and Kawai T 2001 *Phys. Rev. Lett.* **88** 027204

[4] Jin K J, Lu H B, Zhao K, Cheng B L, Chen Z H, Zhou Y L and Yang G Z 2005 *Phys. Rev.* B **71** 184428

[5] Katsu H, Tanaka H and Kawai T 2000 *Appl. Phys. Lett* **76** 3245

[6] Jin K J, Zhao K, Lu H B, Liao L and Yang G Z 2007 *Appl. Phys. Lett.* **97** 081906

[7] Han P, Jin K J, Lu H B, Zhou Q L and Yang G Z 2007 *Appl. Phys. Lett.* **86** 182102

Qiu J, Jin K J, Han P, Lu H B, Hu C L, Wang B P and Yang G Z 2007 *Europhys. Lett.* **79** 57004

Zhou Q L, Jin K J, Lu H B, Han P, Chen Z H, Zhao K, Zhou Y L and Yang G Z 2005 *Europhys. Lett.* **71** 283

[8] Selberherr S 1984 *Analysis and Simulation of Semiconductor Devices* (New York: Springer) chaps 2 & 5

[9] Shockley W and Read W T 1952 *Phys. Rev.* **87** 835

[10] Horio K and Yanai H 1990 *IEEE Trans. Electron Devices* **37** 1093

[11] Huang Y H, Jin K J, Zhao K, Lu H B, He M, Chen Z H, Zhou Y L and Yang G Z 2006 *Chin. Phys. Lett.* **23** 982

[12] Sharma B L and Purosit R K 1974 *Semiconductor Heterojunctions*(Oxford: Pergamon) p 24

[13] Kim M W, Murugavel P, Parashar S, Lee J S and Noh T W 2004 *New J. Phys.* **6** 156

Cohen M I and Blunt R F 1968 *Phys. Rev.* **168** 929