JOURNAL OF APPLIED PHYSICS **103**, 053701 (2008)

Theoretical study on the transport property of p-Si/n-SrTiO$_{3-\delta}$

Chun-lian Hu, Peng Han, Kui-juan Jin,[a] Hui-bin Lu, and Guo-Zhen Yang
Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academic of Sciences, Beijing 100080, People's Republic of China

(Received 2 November 2007; accepted 27 December 2007; published online 4 March 2008)

The transport property of p-Si/n-SrTiO$_{3-\delta}$ heterojunction has been obtained self-consistently with the drift-diffusion model at the temperature range from 200 to 300 K by applying Richardson current at the interface. The band structures, electric field intensities, and carrier distributions at various bias voltages or temperatures are obtained from our calculation. Furthermore, the evolution of the *I-V* behavior with the temperature is also obtained theoretically. From the good agreement between our calculated results and the experimental data, we can conclude that the rectification property in the perovskite-silicon *p-n* junction is owing to the drift-diffusion mechanism and the transport property of Si substrate significantly contributes to the almost linear characteristic of the *I-V* curves. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2890151]

I. INTRODUCTION

Since the high-T_c superconduction and colossal magnetoresistance were observed in the perovskite oxide,[1] much attention has been focused on the novel properties such as ferroelectric, dielectric, ferromagnetic, and superconduction in the perovskite oxides. Owing to these superior properties, the perovskite oxides have been used in many application fields.[2] To combine these excellent properties in the monolithic configuration and to fabricate the oxide intelligent devices, the all-oxide magnetic tunnel junction, *p-n* junctions, field-effect transistors, and superlattices have been studied by many groups.[3–11] Among them, the perovskite-silicon devices, which combine the novel properties of perovskite oxide with the traditional silicon based intelligence, are with great potential application for the next generation of oxide electronics.

As an important perovskite oxide, strontium titanate (SrTiO$_3$), which has a high dielectric constant at room temperature, has been expected to work as the dielectric capacitor in the next generation for dynamic random access memories (DRAM) in very large scale integrated devices.[12,13] To integrate the SrTiO$_3$ DRAM with the Si-based intelligent devices, the excellent p-Si/n-SrTiO$_{3-\delta}$ heterojunction has been fabricated by using the laser molecular-beam epitaxy.[14] In their work, the *I-V* curves of the p-Si/n-SrTiO$_{3-\delta}$ heterojunction show rectification property and almost linear characteristic in bias larger than the threshold value at the temperature range from 200 to 300 K. The slope of the *I-V* curves becomes steeper with the increase of the temperature.

Though the transport property of perovskite-Si heterojunction has been obtained experimentally, the transport mechanism of such a perovskite-silicon *p-n* junction still remain unclear. To reveal the mechanism of the transport property in the silicon based oxide heterojunction, we perform a numerical analysis based on self-consistent calculation of Poisson equation, drift-diffusion formula, and Richardson model[15] in this work. Furthermore, owing to the much larger resistance of the thick substrate of Si than that of SrTiO$_{3-\delta}$, the resistance of the substrate cannot be ignored anymore, which was the case in the system of p-type In-doped and n-type Nb-doped SrTiO$_3$ homogeneous *p-n* junction.[16] So the resistance of the substrate of Si will be also considered as a series resistance here. The good agreement between the measured and calculated *I-V* curves proves that the drift-diffusion model can be employed to analyze the rectification property and the threshold voltages in the system of perovskite-Si *p-n* junction. Furthermore, the transport property of Si substrate plays an important role for the almost linear *I-V* curves of the Si/SrTiO$_{3-\delta}$ heterojunction.

II. MODEL AND METHOD

In this paper, the transport process in the Si/SrTiO$_{3-\delta}$ junction is analyzed on the basis of drift-diffusion model, Poisson equation, carrier continuity equations, and Richardson current at the interface of the *p-n* junction.[15] The electrostatic potential $\varphi(x)$, the concentrations of electrons $n(x)$ and holes $p(x)$ are obtained by solving the coupled current continuity and Poisson equations self-consistently.[16]

In this *p-n* junction, the high density defect states are assumed to be in the band gaps of the p-doped silicon and the n-SrTiO$_{3-\delta}$, thus the so-called Shockley–Read–Hall process dominates the recombination process.[17] The recombination rate is given as

---

[a] Author to whom correspondence should be addressed. Electronic mail: kjin@aphy.iphy.ac.cn.

$$R(x)=\frac{n(x)p(x)-n_i^2}{\tau_{p0}\left[n(x)+n_i\exp\left(\frac{E_t-E_i}{k_BT}\right)\right]+\tau_{n0}\left[p(x)+n_i\exp\left(-\frac{E_t-E_i}{k_BT}\right)\right]},\tag{1}$$

where τ_{p0} and τ_{n0} denote the excess minority carrier hole and electron lifetime, respectively, n_i is the intrinsic carrier concentration, k_B is the Boltzmann constant, T denotes the temperature, E_t is the energy of trapping centers, and E_i is the intrinsic Fermi level.

Expressions for $J_n(x)$ and $J_p(x)$ in the homogenerous regions are given, respectively, by

$$J_n(x)=-q\mu_n n(x)\frac{d\varphi(x)}{dx}+k_BT\mu_n\frac{dn(x)}{dx},\tag{2}$$

$$J_p(x)=-q\mu_p p(x)\frac{d\varphi(x)}{dx}-k_BT\mu_p\frac{dp(x)}{dx},\tag{3}$$

with μ_n and μ_p denoting the mobility of electron and hole, respectively. The current density $J_n(x_I)$ and $J_p(x_I)$ across the interface of the heterojunction x_I are given by[15]

$$J_n(x_I)=A_{+e}^*T^2\exp\left(-\frac{E_c^+-E_{fn}^+}{k_BT}\right)-A_{-e}^*T^2\exp\left(-\frac{E_c^+-E_{fn}^-}{k_BT}\right),\tag{4}$$

$$J_p(x_I)=A_{+h}^*T^2\exp\left(-\frac{E_{fp}^--E_v^-}{k_BT}\right)-A_{-h}^*T^2\exp\left(-\frac{E_{fp}^+-E_v^-}{k_BT}\right),\tag{5}$$

where $A_{e+}^*(A_{h+}^*)$, $A_{e-}^*(A_{h-}^*)$, are the Richardson constants of electron (hole) in the right and left sides of the heterojunction, respectively, E_c^+ and E_v^- are the bottom of conduction band in the n-region and the top of valence band in the p-region, respectively, and $E_{fn}^+(E_{fp}^+)$ and $E_{fn}^-(E_{fp}^-)$ are the quasichemical potentials of conduction band electrons (valence band holes) in the right and left sides of the heterojunction, respectively.

The boundary conditions of Poisson equation are set to be 0 and V_d-V_{bias} at the p and n sides far away from the space charge region, where V_d and V_{bias} denote the built-in potential and the applied bias voltage, respectively. The boundary conditions for the concentration of hole and electron at the p side are N_a and $n_i(0)^2/N_a$, respectively. $n_i(0)$ is the intrinsic concentration at $x=0$. N_d and $n_i(L)^2/N_d$ denote the concentrations of electron and hole at the boundary of n side, respectively, where $n_i(L)$ is the intrinsic concentration in the n region.

Due to the large resistance of the substrate of Si in the p-n junction, the resistance of the substrate cannot be ignored in the calculation. So the total resistance of the p-n junction should be the sum of the junction resistance and the resistance of the substrate. The former is calculated with the drift-diffusion model and the latter is obtained from the experimental data.[14]

III. RESULTS AND DISCUSSION

On the basis of the drift-diffusion model, the energy band diagrams at the bias of 0, ±0.5 V are given in Fig. 1. The space charge region located mostly at the p region of Si as a result of the large concentration of $SrTiO_{3-\delta}$ which is taken as 5.0×10^{19} cm^{-3} while the concentration of Si 1.5×10^{15} cm^{-3} from the Hall effect measurement (Table I).[14]

The distributions of electric field intensity under zero, positive (0.5 V), and reverse (−0.5 V) bias are given in Fig. 2, respectively. As shown in this figure, the electric field intensity under the positive bias is smaller than that with zero bias, while under the reverse bias it is larger than that without bias voltage. The distribution of carriers with various temperatures at 200, 250, and 300 K are plotted in Fig. 3, respectively. In this figure, the minority carrier density increases with the increasing temperatures due to the effect of thermal excitation.

The calculated *I*-*V* curves based on the drift-diffusion model at the temperature range from 200 to 300 K are shown in Fig. 4(a). It can be seen that the rectification property has been obtained, but the theoretical current increases nearly exponentially with the bias voltage above the threshold voltage, while the measured currents shown in Fig. 4(b) increase nearly linearly with the increase of the forward bias. Comparing Fig. 4(a) with 4(b), there is a discrepancy between the calculated and experimental results. As mentioned above, the resistance of the substrate is large enough comparing with the junction resistance. To study the effect of resistance of the substrate on the transport process, the resistance of the substrate of Si is considered as a series resis-

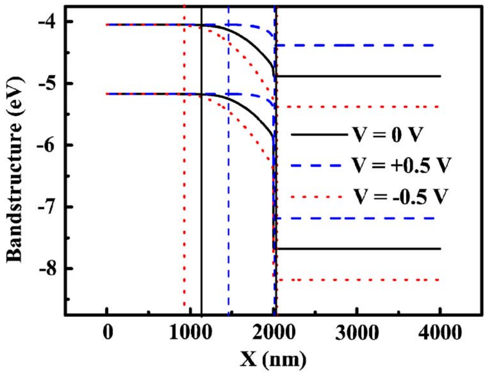

FIG. 1. (Color online) Energy-band diagrams of $Si/SrTiO_{3-\delta}$ at the temperature of 300 K under +0.5, 0, and −0.5 V on the basis of drift-diffusion model. The space charge region is plotted in vertical lines.

TABLE I. The material parameters used in the calculation.

	Si	$SrTiO_{3-\delta}$
Dielectric constant (ε_0)	11.9[a]	300[b]
Electron mobility ($cm^2/V\,s$)	1350[a]	33[c]
Hole mobility ($cm^2/V\,s$)	500[a]	6
Band gap (eV)	1.12[a]	2.8[d]
Electron affinity (eV)	4.05[a]	4.05[e]
Electron lifetime (s)	1.3×10^{-4}[a]	10^{-9}
Bottom of the conduction band (eV)	−4.05	−4.05
Top of the valence band (eV)	−5.17	−6.85

[a] Parameters taken from Ref. 19.

[b] Parameter taken from Ref. 7.

[c] Parameter taken from Ref. 18.

[d] Parameter taken from Ref. 20.

[e] Parameter taken from Ref. 21.

tance in the calculation. The temperature dependence on the substrate resistance of Si obtained from the measurement is represented in Fig. 5. The surface area of the substrate is 10×10 mm^2, and the thickness of it is 1 mm. It can be seen that with the increase of temperature, the resistance of the substrate decreases rapidly. Figure 4(c) shows the calculated *I-V* curves at the temperature range from 200 to 300 K by taking into account the effects of the substrate resistance within the drift-diffusion calculation. It can be seen that the theoretical *I-V* curves in Fig. 4(c) agree much better with the experimental ones in Fig. 4(b). This result demonstrates that the rectification property of the $Si/SrTiO_{3-\delta}$ *p-n* junction is mainly due to the drift-diffusion process and the almost linear *I-V* curve is caused by the transport property of Si substrate. In addition, the increase of forward current with increasing temperatures is mainly contributed by the temperature property of the resistance of Si substrate.

IV. SUMMARY

In summery, the band structures, electric field intensities and carrier densities of perovskite oxide/Si *p-n* junction over a range of temperature from 200 to 300 K have been obtained self-consistently by taking into account the contribution of the Si substrate. The good agreement between the calculated and experimental results of *I-V* curves demonstrates that the rectification property in the perovskite-silicon *p-n* junction is owing to the drift-diffusion mechanism and the transport property of Si substrate significantly contributes to the almost linear *I-V* characteristics of the junction. We believe that the present method should be useful to predict

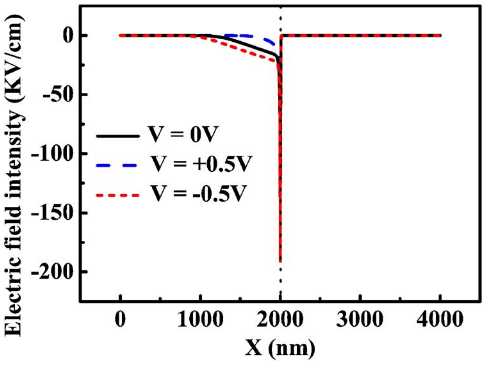

FIG. 2. (Color online) Distributions of electric field intensity in space charge region at various applied bias voltages at the temperature of 300 K of $Si/SrTiO_{3-\delta}$ heterojunction. The interface of the heterojunction is shown in vertical dotted line.

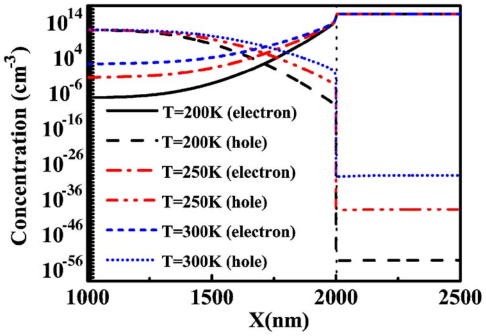

FIG. 3. (Color online) The distributions of the carrier concentrations of *p*-Si/*n*-$SrTiO_{3-\delta}$ junction at zero bias at the temperature of 200, 250, and 300 K, respectively. The vertical dotted line denotes the interface of the *p-n* junction.

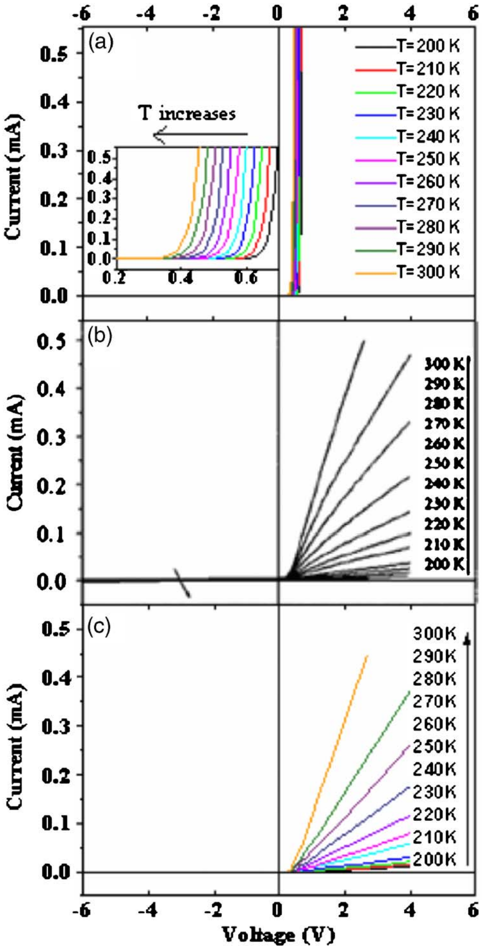

FIG. 4. (Color online) (a)The calculated *I-V* curves of $Si/SrTiO_{3-\delta}$ junction on the basis of the drift-diffusion model over the temperature range of 200–300 K. The inset is the *I-V* curves at the voltage range from 0 to 0.7 V. The temperature range is from 200 K (right) to 300 K (left) at the step of temperature as 10 K. (b) The experimental *I-V* curves of $Si/SrTiO_{3-\delta}$ junction over the temperature range of 200–300 K from Ref. 14. (c) The calculated *I-V* curves of $Si/SrTiO_{3-\delta}$ junction on the basis of the drift-diffusion model by adding a series resistance over the temperature range of 200–300 K.

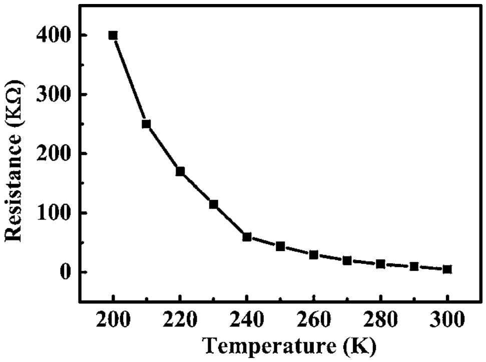

FIG. 5. The temperature dependence of the substrate resistance of *p*-Si. The surface area of the substrate is 10 × 10 mm^2, and the thickness of it is 1 mm.

the property of perovskite-Si *p*-*n* junction for designing promising perovskite/silicon microelectronic devices in the future.

ACKNOWLEDGMENTS

This work has been supported by the National Natural Science Foundation of China and National Basic Research Program of China.

[1] S. Jin, T. H. Tiefel, M. McCormack, R. A. Fastnacht, R. Ramesh, and L. H. Chen, Science **264**, 413 (1994).
[2] M. Sugiura, K. Uragou, M. Tachiki, and T. Kobayashi, J. Appl. Phys. **90**, 187 (2001).
[3] J. Hayakawa, K. Ito, S. Kokado, M. Ichimura, A. Sakuma, M. Sugiyama, H. Asano, and M. Matsui, J. Appl. Phys. **91**, 8792 (2002).
[4] E. T. Wertz and Q. Li, Appl. Phys. Lett. **90**, 142506 (2007).
[5] Y. F. Chen and M. Ziese, Europhys. Lett. **77**, 47001 (2007).
[6] D. Hunter, K. Lord, T. M. Williams, K. Zhang, A. K. Pradhan, D. R. Sahu, and J.-L. Huang, Appl. Phys. Lett. **89**, 092102 (2006).
[7] E. Bellingeri, L. Pellegrino, D. Marre, I. Pallecchi, and A. S. Siri, J. Appl. Phys. **94**, 5976 (2003).
[8] K. Eisenbeiser, J. M. Finder, Z. Yu, J. Ramdani, J. A. Curless, J. A. Hallmark, R. Droopad, W. J. Ooms, L. Salem, S. Bradshaw, and C. D. Overgaard, Appl. Phys. Lett. **76**, 1324 (2000).
[9] J. Kim, Y. S. Kim, and J. Lee, Science **201**, 5374 (2007).
[10] J. C. Jiang, X. Q. Pan, W. Tian, C. D. Theis, and D. G. Schlom, Appl. Phys. Lett. **74**, 2851 (1999).
[11] H. B. Lu, K. J. Jin, Y. H. Huang, M. He, K. Zhao, B. L. Cheng, Z. H. Chen, Y. L. Zhou, S. Y. Dai, and G. Z. Yang, Appl. Phys. Lett. **86**, 241915 (2005); K. J. Jin, H. B. Lu, Q. L. Zhou, K. Zhao, B. L. Cheng, Z. H. Chen, Y. L. Zhou, and G. Z. Yang, Phys. Rev. B **71**, 184428 (2005); Q. L. Zhou, K. J. Jin, K. Zhao, D. Y. Guan, H. B. Lu, Z. H. Chen, and G. Z. Yang, *ibid.* **72**, 224439 (2005); K. J. Jin, H. B. Lu, Q. L. Zhou, K. Zhao, and G. Z. Yang, J. Magn. Magn. Mater. **303**, 329 (2006); K. Zhao, K. J. Jin, H. B. Lu, Y. H. Huang, Q. L. Zhou, M. He, Z. H. Chen, Y. L. Zhou and G. Z. Yang, Appl. Phys. Lett. **88**, 141914 (2006).
[12] A. B. Kozyrev, T. B. Samoilova, A. A. Golovkov, E. K. Hollmann, D. A. Kalinikos, V. E. Loginov, A. M. Prudan, O. I. Soldatenkov, D. Galt, C. H. Mueller, T. V. Rivkin, and G. A. Koepf, J. Appl. Phys. **84**, 3326 (1998).
[13] H. Takashima, R. Wang, N. Kasai, A. Shoji, and M. Itoh, Appl. Phys. Lett. **83**, 2883 (2003).
[14] H. Z. Guo, Y. H. Huang, K. J. Jin, Q. L. Zhou, H. B. Lu, L. F. Liu, Y. L. Zhou, B. L. Cheng, and Z. H. Chen, Appl. Phys. Lett. **86**, 123502 (2005).
[15] M. S. Lundstrom and R. J. Schuelke, IEEE Trans. Electron Devices **30**, 1151 (1983); P. Han, K. J. Jin, Y. L. Zhou, X. Wang, Z. S. Ma, S. F. Ren, A. G. Mal'shukov, and K. A. Chao, J. Appl. Phys. **99**, 074504 (2006).
[16] Q. L. Zhou, K. J. Jin, H. B. Lu, P. Han, Z. H. Chen, K. Zhao, Y. L. Zhou and G. Z. Yang, Europhys. Lett. **71**, 283 (2005).
[17] D. A. Neamen, *Semiconductor Physics and Devices* (McGraw-Hill, New York, 2003).
[18] H. B. Lu, S. Y. Dai, Z. H. Chen, Y. L. Zhou, B. L. Cheng, K. J. Jin, L. F. Liu, G. Z. Yang, and X. L. Ma, Appl. Phys. Lett. **86**, 032502 (2005).
[19] S. M. Sze, *Physics of Semiconductor Devices* (Wiley, New York, 1981).
[20] A. Yoshida, H. Tamura, K. Gotoh, H. Takauchi, and S. Hasuo, J. Appl. Phys. **70**, 4976 (1991).
[21] S. A. Chambers, Y. Liang, Z. Yu, R. Droopad, J. Ramdani, and K. Eisenbeiser, Appl. Phys. Lett. **77**, 1662 (2000).