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A Theoretical Study of Transport Property of Heterojunction and Evaluation of Electric Fields of The Space Charge Region and Energy Band of The Heterojunction Under Applied Bias Voltage

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ABSTRACT

This paper presents a theoretical study of transport property of heterojunction and evaluation of electric fields of the Space charge region and energy band of the heterojunction under applied bias voltage. The study exhibits a typical XRD pattern of a 500 thick LSMO film growing directly on the Si (001) substrate. The plane lattice parameter is about 5.43 A° for Si. and about 3.86 A° for LSMO. With the LSMO unit cell rotating 45 around the S 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. The study 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 exponential data clearly present asymmetric f-V curves of the LSMO/Si heterojunction 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. 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.

Keywords:- Heterojunction, Bias Voltage, Space Charge, Energy Band, Degree of freedom

I. INTRODUCTION

Perovskite manganese oxides La]_xAxMn03 (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^Aj^MnOg, such as double exchange theory,2 phase separation mechanism3 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 magneto resistance from interface effect,5 and photovoltaic effect5 have been reported. Integrating the perivskite-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 La0 7SrQ gMnOg/Si (LSMO/Si) p-n juntions.7 One also reported the transport property of the LSMO/Si heterojunction.6 However, no corresponding theoretical work has been reported so far. Generally speaking, the en

electrons in perovskite manganese oxides were though to be localized in the perovskite manganese oxide because of the strong Hund's rule coupling between the eg electrons and t2g electrons, and the eg 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 of SrTiOg/Si (001) interface, and revealed the characteristics of the band structure of SrTiOg/Si.0 Our early theoretical work also confirmed that the band picture can interpret the transport property of the SrTi03/Si p-n homojunction.10 In order to further investigate the application of band scenario to the transport property of heterostructure based on perovskite manganese oxides One presents 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 coupling among charge, spin and orbital degrees of freedom.

II. EXPERIMENTAL RESULTS

The LSMO/Si heterojunction were obtained by depositing 500 nm thick LSMO films (work function of 4.96 eV)11 and band gap of 1.0 eV12 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. 0-2 0 X-ray diffraction was carried out to examine the crystalline quality of the LSMO thin film on a Si (001) substrate, the results of which are shown in Fig. 4.1. To measure the transport characteristics of the LSMO/Si heterojunction, indium (In) electrodes (2*2 mm2) were symmetrically attached the surface of the LSMO film and of the Si water as shown in the inset of Fig. 4.2. The current-voltage

III. MATHEMATICAL FORMULAE USED IN THE EVALUATION

To gain the insight into the nature of the transport property at the interface region of the heterostructure, one 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 :

$$\frac{d2\psi(x)}{dx2} = (q/\varepsilon)(p(x)\text{-}n(x)+N \qquad (4.1)$$

where ψ (x) is the electric potential, q is the elementary charge, 8 is the permittivity of a semiconductor which is taken as 10 for LSMO15 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 1020cm“3 for LSMO from our Hall measurement and 1016cm-3 for Si.13 For the one-dimensional case under a steady state the continuity equations

$$q(G_n(x)\text{-}U_n(x)) + \frac{dJn}{dx} = 0$$
$$q(G_p(x)\text{-}U_p(x)) + \frac{dJp}{dx} = 0 \qquad (4.2)$$

where Gn(x) and Gp(x) are the electron and hole generation rate, respectively, Un(x) is the electron recombination rate in p-type semiconductor, and Up(x) is the hole recombination rate in n-type semiconductor rate in n-type semiconductor. Jn and Jp are the electron current density and the hole current density respectively, which can be which can be described as follows

$$J_n = -q\mu_n\left(n(x)\frac{d\psi(x)}{dx} - (kT/q)\frac{d\psi(x)}{dx}\right)$$

$$J_p = -q\mu_p\left(p(x)\frac{d\psi(x)}{dx} + (kT/q)\frac{dp(x)}{dx}\right)$$

where p is the hole mobility which is taken as 500 cm2/V.s for Si13 and 1.8 cm2/V.s for LSMO from our Hall measurement. un the electron mobility which is taken as 10 cm2/V.s for LSMO and 1359 cm2/V.s for Si,13 and the parameter k and T are Boltzmann constant and the ambient temperature,'respectively. The electron effective mass is taken as 1.06 me, for Si.13 The effective mass for LSMO is taken as 4 mc.15 The parameter me is the free electron rest mass. Using boundary condition of various bias voltages and self-consistency solving Poisson's equation (4.1) and the current-continuity equation (4.2) by using Newton's iteration method and the uncoupled method, one 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.

IV. RESULTS AND DISCUSSION

The study exhibits a typical XRD pattern of a 500 nm thick LSMO film growing directly on the Si (001) substrate. Except for (001) 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 (001) direction. This result can be understood as follows. The inplane lattice parameter is about 5.43 A for Si, and about 3.86 A for LSMO. With the LSMO unit cell rotating 45 around the S surface normal (100) axis, the lattice mismatch between LSMO and Si is about 0.55 %. The small lattices' mismatch allows a nearly epitaxial growth of LSMO on Si substrate.

The study presents the experimental and theoretical results of 7-1/ 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, one introduces series resistance into the calculation I-V characteristics. The series resistance was taken as 2kT2, 2.5 kQ and 3.8 kQ 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 one 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 Si02 between Si substrate and epitaxial LSMO film on the transport properties of

LSMO/Si heterojunction in this thesis. 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. 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 denoted the position of the interface of the LSMO/Si rojunction. Figure 4.3 shows that the potential barrier of the LSMO/Si heterojunction decrease under a forward bias and increases under a reverse bias. One can also see that the space charge region mainly located in the n-Si region, which is caused by the much smaller carrier concentration of Si than that of LSMO. Figure 4.4 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. The maximum magnitude of the electric field under various biases exists at the interface of the LSMO/Si heterostructure. In table 4T1 and 4T2, we have shown the electricfields of the space charge and calculated eneregy band of the LSMO/Si heterojunction obtained by solving eq. (4.1) and (4.2) under bias voltage.

In summary, the transport characteristics of 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 shows 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.[16-20]

Table T1

An Evaluation results of electric fields of the space charge region of LSMO/Si heterojunction obtained by solving eq. (4.1) and (4.2) under applied voltage OV, 0.4 V and - 0.4 V

X (nm)	Electric field (KV/ nm)		
	-0.4 V	0.0 V	-0.4 V
900	0.002	0.006	0.008
1000	0.004	0.017	0.020
1000	-0.015	-0.058	-0.067
1200	- 0.250	- 0.127	- 0.228
1300	-0.360	- 0.273	- 0.143
1400	- 0.380	- 0.148	- 0.128
1500	- 0.226	- 0.122	- 0.087
1600	- 0.167	-0.095	0.043
1700	- 0.105	0.028	0.182
1800	-0.092	0.047	0.227
1900	0.028	0.088	0.320
2000	0.005	0.122	0.435 .

Table T2

An Evaluation of band sup (V) of the LSMO/^i heterojunction under applied bias voltage OV, 0.4 V and - 0.4 V

X (nm)	Electric field (KV/nm)		
	0 V	0.4 V	-0.4 V
200	- 4.05	-4.00	- 4.105
300	-4.005	-4.00	- 4.133
400	- 4.05	- 4.000	- 4.147
500	- 4.05	-4.00	- 4.188
600	- 4.05	- 4.00	- 4.212
700	-4.05	-4.00	- 4.237
800	- 4.05	- 4.00	- 4.248
900	- 4.07	-4.00	- 4.250
1000	- 4.52	- 4.05	- 4.276
1200	- 5.15	- 4.22	- 4.298
1400	- 5.35	- 4.34	- 4.386
1600	- 5.52	- 4.39	- 4.433
1800	- 5.78	- 4.44	- 4.476
2000	- 6.00	- 4.50	- 4.536

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