Energy Levels in Si and $SrTiO_3$-Based Quantum Wells with Charge Image Effects

T. A. S. Pereira, M. G. Bezerra, J. A. K. Freire, V. N. Freire, and G. A. Farias
Departamento de Física, Universidade Federal do Ceará,
Campus do Pici, Caixa Postal 6030, 60455-900 Fortaleza-CE, Brazil

Received on 4 April, 2005

In the present work we develop a theoretical study to analyze how the image charges effects can modify the electronic properties in *Si* and $SrTiO_3$-based quantum wells. We have used the method based on the calculation of the image charge potential by solving Poisson equation in cylindrical coordinates. The numerical results show that the electron-heavy hole recombination energy can be shifted by more than 200 meV due to the combination of charge image and SiO_2 ($SrTiO_3$) interface thickness effects.

Keywords: Energy Levels; Si; $SrTiO_3$-based quantum wells

I. INTRODUCTION

The SiO_2 gate thickness shrinkage to less than 50 Å is driving research efforts to find alternative oxides with high-k dielectric constant to allow for physically thicker films that can limit leakage current problems [1]. Recent research shows that $SrTiO_3$, HfO_2 and TiO_2 materials are the most promising candidates to SiO_2 replacement in development of new semiconductors devices. With the advances in the growth of $SrTiO_3$ on silicon by epitaxy [2], the development of quantum confinement based optical devices is possible, following the steps of an original suggestion and demonstration of light emission in Si/SiO_2 quantum wells (QWs) [3, 4], by simple replacement of silicon dioxide by $SrTiO_3$. The understanding of the atomic structure at the *silicon/oxide* interface is still not complete. However, the ability to grow gate quality crystalline oxide films on *Si* in industrial scale is yet to be demonstrated. Droopad *et al*. [5] observed that the possible explanation for the formation of such an amorphous layer includes the diffusion of oxygen during the growth of the oxide layer reacting with the interfacial *Si* atoms. This would suggest that the interface layer is some form of SiO_x with $x \leq 2$. Chambers *et al.* [6] have shown that the interest in including an interfacial layer of SiO_2 suggests significant progress in order to reduce the leakage current, either because SiO_2 acts as an electron tunnel barrier or because SiO_2 at the interface increases the conduction band offset between $SrTiO_3$ and *Si*. Tuan *et al*. [7] show that the TiO_2 can not be grown directly on *Si* because of thermodynamic instabilities, leading to $TiSi_x$ and SiO_2 at the interface. However, TiO_2 can be grown as an epitaxial film on $SrTiO_3$ (001) that can be grown epitaxially on *Si*(001) with negligible interface reaction.

In this work, we present results on electron–hole energy recombination from confined states in abrupt $Si/SiO_2/SrTiO_3$ and $Si/SrTiO_3/TiO_2$ QWs. The aim is to search for high-*k* dielectric based light emission devices, which can be important in developing silicon-based technology for future nano-optoelectronic device integration. The dielectric mismatches among the materials of QWs are included through the conventional image potential for a point charge Q near an interface [8].

II. THEORETICAL MODEL

The carrier Hamiltonian in Si and $SrTiO_3$-based quantum wells can be written as

$$H(z) = -\frac{\hbar^2}{2}\frac{d}{dz_i}\left(\frac{1}{m_i}\frac{d}{dz_i}\right) + V_T(z), \tag{1}$$

with i = electron or hole and the total effective potential $V_T(z)$ given by

$$V_T(z) = V_0(z) + V_{im}(z), \tag{2}$$

where $V_0(z)$ is the potential energy due to the conduction (or valence) band offset and $V_{im}(z)$ is the image charge potential contribution, given by the Poisson's equation due to the presence of a point charge

$$\vec{\nabla}\cdot\left[\varepsilon(z)\vec{\nabla}\phi(\vec{r})\right] = -Q\delta(\vec{r}-\vec{r}_0). \tag{3}$$

The solution in the cylindrical coordinates is independent of the azimuth angle φ (see detail in Ref. [8]). In this case, we can write $\phi(\vec{r})$ in the general form

$$\phi(\vec{r}) = \int_0^\infty qJ_0(qR)A_q(z)dq, \tag{4}$$

where $J_0(qR)$ is the Bessel function of the zeroth order, $A_q(z)$is a function determined by the boundary conditions of $\phi(\vec{r})$ at the interfaces. The solution for the image potential $V_{im}(z)$ is

$$V_{im}(z_0) = \frac{Q}{2}\int_0^\infty q\left[A_q(z_0) - A_q^0(z_0)\right]dq, \tag{5}$$

where $A_q^0(z_0)$ is solution of (3) if the dielectric constant were z independent.

Using the above considerations, we solved the Schrödinger equation for the perpendicular motion:

$$H_i(z_i)\psi_i(z_i) = E_i^n\psi_i(z_i) \qquad (6)$$

and the eigenvalues and eigenfunctions of this equation are calculated through a matrix transfer scheme [9].

III. NUMERICAL RESULTS

The heterostructures used in our simulations have been a $TiO_2/SrTiO_3/Si$ and $SrTiO_3/SiO_2/Si$ QW. All the parameters used for $SrTiO_3$, SiO_2, TiO_2 and Si are presented in Table I.

TABLE I: Parameters of the materials used in our theoretical calculations [10-12].

	Si	SiO_2	$SrTiO_3$	TiO_2
E_g (eV)	1.1	8.9	3.3	3.2
$\varepsilon/\varepsilon_0$	11.7	2.1	300	100
$m_{e,\perp}/m_0$	0.173	0.3	0.676	0.3454
$m_{hh,\perp}/m_0$	0.533	5.0	1.588	5.0208

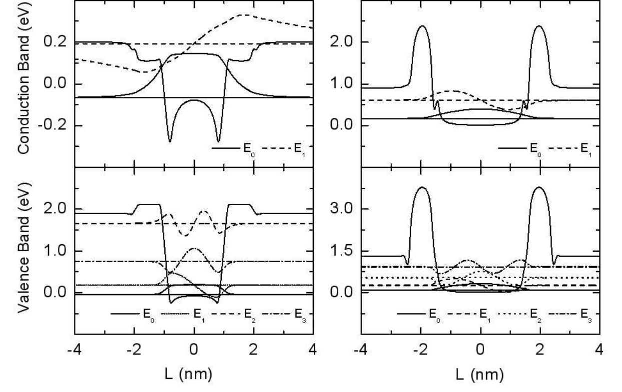

FIG. 1: Confinement $V(z) = V_0(z) + V_{im}(z)$ potentials for 50 Å wide $TiO_2/SrTiO_3/Si$ (left) and $SrTiO_3/SiO_2/Si$ (right). Energy levels and wave function are also depicted.

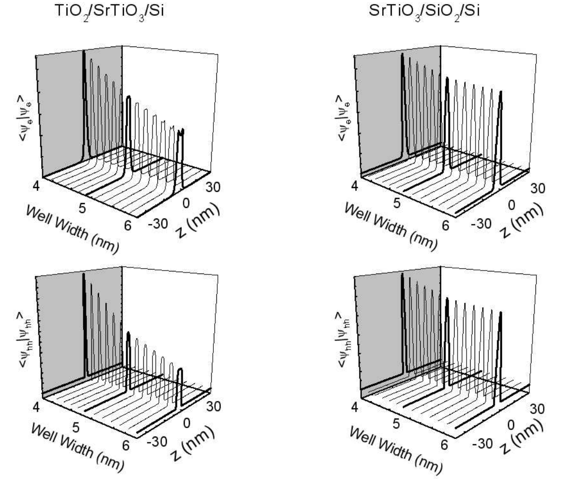

FIG. 2: Electron (top) and heavy hole (bottom) ground states wave functions confined in abrupt $TiO_2/SrTiO_3/Si$ and $SrTiO_3/SiO_2/Si$ QWs, with well width of 4 to 6 nm.

In the present calculation two effects are considered, the charge image and the interface thickness. Fig. 1 shows the confinement potential $V_T(z)$ and the wave functions of $TiO_2/SrTiO_3/Si$ (left) and $SrTiO_3/SiO_2/Si$ (right) heterostructures with quantum well width of 5.0 nm and SiO_2 ($SrTiO_3$) layers with thickness of 1.0 nm.

Considering $TiO_2/SrTiO_3/Si$ system, and based on the work of Tuan *et al.* [7], the conduction band offset of 0.1 eV and 0.2 eV between Si and $SrTiO_3$ and between Si and TiO_2, respectively were used – see Fig. 1 (left). In this structure the attractive character of the image charges in the well region introduce a sharp and deep potential profile which can trap carriers close to the SrTiO3/Si interfaces. This fact can be seen looking through the top of electron wave function evolution in Fig. 2 (left).

For $SrTiO_3/SiO_2/Si$ systems electron confinement was not observed if we consider a band offset of 0.1 eV between $SrTiO_3$ and Si. In this structure we have used a band offset of 0.9 eV, as proposed by Zang *et al.* [13]. Thus, as shown in Fig. 1 (right), there are two confined states for electrons and four confined states for heavy hole in a narrow QW with width of 5.0 nm. We also observed that in this system the SiO_2/Si interface does not permit interfacial confinement due to the repulsive character of the image charge in the well region – see Fig. 2 (right).

Figure 3 shows the results for electron-heavy hole recombination energy in $TiO_2/SrTiO_3/Si$ QW (top) and $SrTiO_3/SiO_2/Si$ QW (bottom), as function of the QW width for $SrTiO_3$ (SiO_2) layer with thickness of 1.0 nm and 1.5 nm. Solid and dashed lines represent carrier recombination energy including the effects due to image charges.

Dashed dotted and dotted lines represent carrier recombination energy without image charges effects. The attractive character of the image potential in the well region of $TiO_2/SrTiO_3/Si$ QW, Fig. 3 (top), decreases the recombination energy (solid and dashed lines), when compared with carrier recombination energy in QW without image charge effect (dashed dotted and dotted lines). The repulsive image potential in the well region of $SrTiO_3/SiO_2/Si$ QW, Fig. 3 (bottom), increases the recombination energy. The $SrTiO_3$ (SiO_2) layer is expressive because it strongly affects the recombination energy of the QWs. Fig. 3 also shows that increasing the thickness of the $SrTiO_3$ (SiO_2) layer, the recombination energy blue-shift in $TiO_2/SrTiO_3/Si$ by about 40 meV and in $SrTiO_3/SiO_2/Si$ by about 800 meV, respectively, for a well width of 4.0 nm.

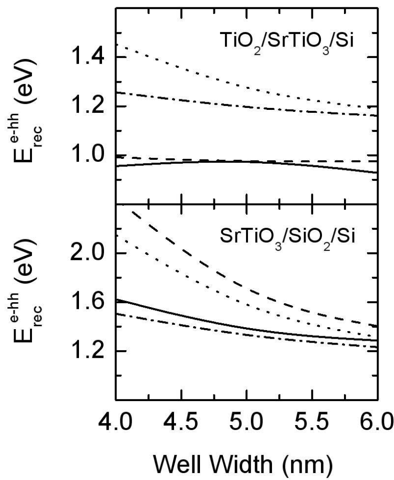

FIG. 3: Electron-heavy hole recombination energy in (top) $TiO_2/SrTiO_3/Si$ and (bottom) $SrTiO_3/SiO_2/Si$, as a function of the well width and $SrTiO_3$ (SiO_2) layer with thickness of 1.0 nm (solid and dashed dotted lines) and 1.5 nm (dashed and dotted lines).

In conclusion, we have studied image charges effects in $TiO_2/SrTiO_3/Si$ and $SrTiO_3/SiO_2/Si$ QWs. The image charges related potential structure (sharp and deep) can trap electrons close to the $SrTiO_3/Si$ interfaces. In this system we also observed that the attractive character of the image potential inside of the well region decreases the recombination energy. For $SrTiO_3/SiO_2/Si$ QW we observed electron confinement only for a 0.9 eV conduction band offset between the $SrTiO_3$ and Si layers. This structure does not have a sharp and deep potential profile due to the repulsive character of the image potential that increases the recombination energy, consequently the carrier do not presents an interfacial confinement.

Acknowledgement

T. A. S. Pereira and M. G. Bezerra were supported by Brazilian National Research Council (CNPq). The authors also would like to acknowledge the NanoSemiMat #550.015/01-9.

[1] J. Robertson, J. Vac. Sci. Technol. B **18**, 1785 (2000).
[2] S. Migita, S. Sakai, J. Appl. Phys. **89,** 5421 (2001).
[3] R. Tsu, Nature **364**, 19 (1993).
[4] Z. H. Lu, D. J. Lockwood, J. -M. Baribeau, Nature **378**, 258 (1995).
[5] R. Droopad, Z. Yu, J. Ramdani, L. Hilt, J. Curless, C. Overgaard, J. L. Edwards, J. Finder, K. Eisenbeiser, J. Wang, J. Wang, V. Kaushik, B-Y Ngyuen, B. Ooms, J. Cryst. Growth **227/228**, 936 (2001).
[6] S. A. Chambers, Y. Liang, Z. Yu, R. Droopad, and J. Ramdani, J. Vac. Sci. Technol. A **19,** 934 (2001).
[7] A. C. Tuan, et al., App.Phys. Lett. **83**, 3734 (2003).
[8] T. A. S. Pereira, E. W. S. Caetano, J. A. K. Freire, V. N. Freire, and G. A. Farias, Brazilian Journal of Physics **34**, 684 (2004).
[9] J. A. K. Freire,G. A. Farias, and V. N. Freire, Solid State Commun. **106**, 559 (1998).
[10] G. Theodorou, G. Tsegas, P. C. Kelires, E. Kaxiras, Phys. Rev. B **60**, 11494 (1999); J. R. Chelikowsky and M. Schluter, Phys. Rev. B **15**, 4020 (1997).
[11] B. Brar, G. D. Wilk, A. C. Seabaugh, Appl. Phys. Lett. **69**, 2728 (1996).
[12] M. Marques, L. K. Teles, V. Anjos, L. M. R. Scolfaro, J. R. Leite, V. N. Freire, G. A. Farias, E. F. da Silva Jr., Appl. Phys. Lett. **82**, 3074 (2003).
[13] X. Zhang, A. A. Demkov, Hao LI, X. Hu, and Yi Wei, Phys. Rev. B **68**, 125323 (2003).