Energy Levels in Si and SrTiO$_3$-Based Quantum Wells with Charge Image Effects

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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-κ 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 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$_2$ 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-κ dielectric based light emission devices, which can be important in developing silicon-based technology for future optoelectronic device integration. The dielectric mismatch 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

\[ H(z) = -\frac{\hbar^2}{2} \frac{d}{dz} \left( \frac{1}{m_0} \frac{d}{dz} \right) + V_T(z), \] (1)

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

\[ V_T(z) = V_0(z) + V_{im}(z), \] (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

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

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

\[ \phi(\vec{r}) = \int_0^\infty J_0(qR)A_q(z) dq, \] (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

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

where $A_q'(z_0)$ is solution of (3) if the dielectric constant were $z$ independent.
Using the above considerations, we solved the Schrödinger equation for the perpendicular motion:

\[ H(z_i)\psi_i(z_i) = E_i \psi_i(z_i) \]  

(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].

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>SiO(_2)</th>
<th>SrTiO(_3)</th>
<th>TiO(_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E(_g) (eV)</td>
<td>1.1</td>
<td>8.9</td>
<td>3.3</td>
<td>3.2</td>
</tr>
<tr>
<td>(E/\varepsilon_0)</td>
<td>11.7</td>
<td>2.1</td>
<td>300</td>
<td>100</td>
</tr>
<tr>
<td>(m_e/m_0)</td>
<td>0.173</td>
<td>0.3</td>
<td>0.676</td>
<td>0.3454</td>
</tr>
<tr>
<td>(m_{hh}/m_0)</td>
<td>0.533</td>
<td>5.0</td>
<td>1.588</td>
<td>5.0208</td>
</tr>
</tbody>
</table>

In the present calculation two effects are considered, the charge image and the interface thickness. Fig. 1 shows the confinement potential \(V(z)\) 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 introduces a sharp and deep potential profile which can trap carriers close to the SrTiO\(_3\)/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) $\text{TiO}_2/\text{SrTiO}_3/\text{Si}$ and (bottom) $\text{SrTiO}_3/\text{SiO}_2/\text{Si}$, as a function of the well width and $\text{SrTiO}_3$ ($\text{SiO}_2$) 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 $\text{TiO}_2/\text{SrTiO}_3/\text{Si}$ and $\text{SrTiO}_3/\text{SiO}_2/\text{Si}$ QWs. The image charges related potential structure (sharp and deep) can trap electrons close to the $\text{SrTiO}_3/\text{Si}$ 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 $\text{SrTiO}_3/\text{SiO}_2/\text{Si}$ QW we observed electron confinement only for a 0.9 eV conduction band offset between the $\text{SrTiO}_3$ and $\text{Si}$ 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.