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<th>Strain profile, electronic band structure and optical gain of self-assembled Ge quantum dots on SiGe virtual substrate (Conference main paper 4 pages long)</th>
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<td><strong>Author(s)</strong></td>
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Strain Profile, Electronic band structure and Optical Gain of self-assembled Ge quantum dots on SiGe virtual substrate


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1. Introduction

Group IV (Si, Ge, Sn) alloys are promising materials for future optoelectronic devices. Their compatibility with Si technology would allow us to engineer novel growth techniques and bandgap engineering methods to obtain direct band gap materials [1]. Other alloy compositions could allow wider wavelength range [2] which can revolutionize the photonics industry - leading to new design of LEDs, photodetectors, laser diodes and electro optical modulators.

In this paper, we study one such possible structure - self assembled Ge QDs embedded on Si₀.₅Ge₀.₅ virtual layer with the same capping layer. A wetting layer is considered to simulate the actual scenario. Then we conduct a theoretical study on the strain and electronic band structure of this model. We employ the valence force field (VFF) method using Keating potential to estimate the strain followed by 8 band k\cdot p method to calculate the electronic band structure taking the \Gamma valley into consideration. Finally we study the optical gain of the system for varying carrier concentrations.

2. Computational Methods

2.1. Valence Force Field Strain Calculation

We use the VFF method with the Keating potential [3] to calculate the strain energy, \( E_{\text{strain}} \) expressed in terms of the bond lengths and bond angles as

\[
\begin{align*}
E_{\text{strain}} & = \frac{1}{2} \sum_{i,j} \left( \frac{3a_{i-j}}{8a_{0,i-j}} \left( \left| x_i - x_j \right|^2 - d_{0,i-j}^2 \right) \right) + \\
& + \sum_{i,k} \left( \frac{3\beta_{i-k}}{8d_{i,i-k}^2} \cdot \left[ \left| x_i - x_k \right| \cdot \left| x_i - x_k \right| \left| x_i - x_k \right| \right] + \\
& + \frac{1}{3} \left( a_{0,i-j} \right) \left( d_{0,i-j} \right) \left( d_{0,i-j} \right) \right)^2
\end{align*}
\]

Here the first summation runs over all atoms \( i \) and their four nearest neighbors \( j \); the second summation runs over all atoms \( i \) and their pairs of neighbors \( j \) and \( k \). \( x_i \) is the position vector of the \( i^{th} \) atom and \( d_{0,i-j} \) is the strain free bond length of the \( i - j \) bond related to the strain free \( i - j \) lattice constant \( a_{0,i-j} \) as per the relation \( d_{0,i-j} = (\sqrt{3}/4)a_{0,i-j} \). \( a_{0,i-j} \) is the bond stretching force constant of the \( i - j \) bond, and \( \beta_{i-k} \) is the bond bending force constant of the \( j - i - k \) bond angle [3]. Values used in our calculation are from Ref. [4]. Our intention is to minimize \( E_{\text{strain}} \) and let the system attain a stable state, thus we allow each atom to vibrate and move along the direction of force acting on it. The force on the \( i^{th} \) atom is given by \( F_i = -\nabla_i(E_{\text{strain}}) \). This is continued until there is no more force acting and all the atoms have settled down [3]. Now the energy-minimized final position of each atom is compared with its initial strain-free location to obtain the strain profile of the final system.

2.2. 8 band k\cdot p calculation

We use the 8 band \( k\cdot p \) method to calculate the electronic band structure for the \( \Gamma \) valley. 6 band \( k\cdot p \) method [5] is not very reliable to study Ge as it does not consider the interaction between the conduction band (CB) and valence band (VB). On the other hand 15 band \( k\cdot p \) [5] is ideal to study the full extent of the Brillouin zone at the expense of introducing many fitting parameters. In this work, we use the 8 band \( k\cdot p \) which is accurate enough to study the subband energy dispersion curves near the \( \Gamma \) point of the [001] oriented Ge/Si₀.₅Ge₀.₅ strained QDs. The Hamiltonian for the strained QD can be simply written as [6]

\[ H = H_k + \sum_{\sigma} V_{\sigma}(z) + H_s \]  (2)

For simplicity \( H \) is split into three components, the first being \( H_k \) which stands for the kinetic 8-band effective-mass Hamiltonian. This can incorporate the interaction between the CB and the VB; and the spin-orbit (SO) coupling within the VB. The second term \( V_{\sigma}(z) \) accounts for the band offset effects in the strain-free condition, whereas the third term \( H_s \) stands for the strain induced Hamiltonian. The \( 8\times8 \) expansion of the Hamiltonian matrices can be referred to our in previous work [6]. The material parameters used in the \( k\cdot p \) calculation the same used in our recent work [7].
2.3. Optical Gain Calculation

In this work we take account both homogenous and inhomogeneous broadening of the optical gain spectrum. The expression for the gain is given by [8]

\[ G(E) = \frac{\pi e^2 h}{m_0^2 n_r e_0 c E} \sum_{n_c n_v} \frac{[M_{cv}^2][f_c + f_v - 1]}{V} \times \frac{B_{cv}(E - E_{cv})}{\pi} \] (3)

where \( E \) is the photon energy, \( e \) is the electronic charge, \( n_r \) is the refractive index of the QD material, \( e_0 \) is free-space dielectric constant, \( E_{cv} \) is the transition energy, and \( f_c \) and \( f_v \) are the CB and VB Fermi-Dirac distributions respectively given by Eq. (4) and (5).

\[ f_c = \frac{1}{1 + \exp[(E_{nc} - E_{fc})/k_B T]} \] (4)

\[ f_v = \frac{1}{1 + \exp[(E_{nv} - E_{fv})/k_B T]} \] (5)

where \( E_{nc} \) and \( E_{nv} \) are the quantized electron and hole energy level respectively; and \( E_{fc} \) and \( E_{fv} \) are the electron and hole quasi-Fermi level respectively. In the gain calculation, \( M_{cv}^2 \) is one of the most important parameters which is the optical transition matrix element. The squared optical transition matrix element measures the momentum of the transition between the hole subband and the electron subband [9]

\[ M_{cv}^2 = \langle \Psi_{n-x,k} | \hat{p}_i | \Psi_{n+y,k} \rangle, \quad i = x, y, z \] (6)

where \( \hat{p}_i \) stands for the momentum operator; and \( \Psi_{n-x,k} \) and \( \Psi_{n+y,k} \) represent the real electron and hole wavefunctions respectively. Detailed expressions of the optical transition matrix elements can be found in our previous work [8].

3. Results and Discussion

For the Ge/Si_{0.5}Ge_{0.5} QD, we assume the pyramid growth is along +z direction, the base and wetting layer are in the x-y plane. The wetting layer is two monolayer thick. Fig. 1 shows the front view schematic of the QD structure with grayscale legends. The wetting layer is not shown for sake of simplicity.

Our pyramidal QD is of height \( (h) = 18 \times \) lattice constant and base \( (2h) = 36 \times \) lattice constant. The entire system’s height is \( 3h \) and the length/width is \( 4h \), which will be clear from Fig 1 and 3.

Before proceeding into the strain profile examination we lay down few more labels, as can be seen in Fig. 3. It shows the top view of our QD system with labels consistent with Fig. 2. Additionally we label the centers of the top ABCD, wetting layer JKLM and base PQRS as E, O and T respectively. These labels will prove to be helpful to describe the various strain profiles that follow.

Table I. shows the list of strain profile examined in this work with their description, type and figure number.
Table 1. List of Strain Profiles with description

<table>
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<th>Profile</th>
<th>Description</th>
<th>Type</th>
<th>Fig. No.</th>
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<tr>
<td>(a)</td>
<td>Along [001] through E,O,T</td>
<td>1D</td>
<td>4</td>
</tr>
<tr>
<td>(b)</td>
<td>Along [010]/[100] through QD center (z = 1.5h)</td>
<td>1D</td>
<td>5</td>
</tr>
<tr>
<td>(c)</td>
<td>( \varepsilon_{xx} ) in JKLM (001) x-y plane</td>
<td>2D</td>
<td>6</td>
</tr>
<tr>
<td>(d)</td>
<td>( \varepsilon_{yy} ) in JKLM (001) x-y plane</td>
<td>2D</td>
<td>7</td>
</tr>
<tr>
<td>(e)</td>
<td>( \varepsilon_{zz} ) in JKLM (001) x-y plane</td>
<td>2D</td>
<td>8</td>
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In Fig. 4, \( \varepsilon_{xx} / \varepsilon_{yy} \) (\( \varepsilon_{zz} \)) increases (decreases) monotonically in the substrate and jumps to about -0.016 (+0.003) at the QD interface (wetting layer). Within the QD \( \varepsilon_{xx} / \varepsilon_{yy} \) (\( \varepsilon_{zz} \)) increases (decreases), with a sudden jerk again at the interface changing sign (i.e. strain type). Finally in the capping layer both fall to zero. This result is consistent with [4].

Fig. 5 shows the strain profile along the [010] and [100] direction in the same plot. \( \varepsilon_{xx} \) in the [010] direction is identical to \( \varepsilon_{yy} \) in the [100] direction; and vice-versa. \( \varepsilon_{zz} \) is the same in both cases. In the center of the QD, \( \varepsilon_{xx} \) and \( \varepsilon_{yy} \) are exactly the same in both
Fig. 7 shows the contour plot of $\varepsilon_{xy}$ in the JKLM (001) wetting layer $x$-$y$ plane with legends and labels. Fig. 6 and Fig. 7 can be easily correlated as $\varepsilon_{xx}$ in the [010] direction is identical to $\varepsilon_{yy}$ in the [100] direction and $\varepsilon_{xy}$ in the [010] direction is identical to $\varepsilon_{xx}$ in the [100] direction. This idea is very clear from the comparison of the two plots in Fig. 6 and 7.

Fig. 8 shows the contour plot of $\varepsilon_{zz}$ in the JKLM (001) wetting layer $x$-$y$ plane. It clearly shows that there is very less strain outside the QD, but at the QD boundaries. It is greater outside the base edges and even greater within the base of the pyramidal QD.

3.2. Energy level
The energy profile of the $\Gamma$ point is shown in Fig. 9. It also shows the degeneracy in each energy level. The fundamental transition energy is 1301.14 meV (952.89 nm).

![Energy profile of the $\Gamma$ point](image)

**Fig. 9.** Calculated energy level at the $\Gamma$ point

3.3. Optical Gain
In Fig. 10, the optical gain is compared for varying injection carrier concentrations.

![Gain vs. Transition Energy](image)

**Fig. 10.** Gain vs. Transition energy for varying injection carrier concentration

The injection carrier concentrations is varied across 1, 2, 4, 6 and $8 \times 10^{18}$ cm$^{-3}$ and labeled in the plot. For $1 \times 10^{18}$ cm$^{-3}$ there is no gain and it steadily increases with increase in injection carrier concentration. For this calculation only the $\Gamma$ valley was considered. Future calculations would take into account also the interaction and effect from the $L$ valley.

4. Conclusion
In this work we study the strain profile using VFF theory, energy levels using 8 band $k\cdot p$ method and optical gain of Ge quantum on SiGe virtual substrate. The strain-induced energy shift in the quantum is proportional to $(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$ which justifies the need to study the strain profile in such depth. This was followed by calculation of energy level and optical gain. The fundamental transition energy was found to be 1301.14 meV (952.89 nm). The optical gain starts improving for injection carrier concentrations over $1 \times 10^{18}$ cm$^{-3}$. However in this calculation only the $\Gamma$ valley was considered and future work would also consider the $L$ valley.

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References