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# Strain Profile and Size Dependent Electronic Band Structure of GeSn/SiSn Quantum Dots for Optoelectronic Application

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**Abstract:** We study self-assembled GeSn/SiSn quantum dots for optoelectronic application in the Silicon photonics domain. Valence force field and  $k \cdot p$  methods are used to investigate the strain distribution and band structure with size effect.

## 1. Introduction

The compatibility of group IV elements with Si CMOS fabrication technology has enabled us to integrate both optical and electronic components onto a single microchip [1] providing faster optical data transfer both between and within microchips. Quantum Dot (QD) based optoelectronic devices could be a key enabler in this domain of research. In this paper, we study one such possible structure - self assembled Ge<sub>0.5</sub>Sn<sub>0.5</sub> QDs embedded on Si<sub>0.5</sub>Sn<sub>0.5</sub> substrate/cap with wetting layer. Valence force field (VFF) method using Keating potential is employed to estimate its strain profile followed by electronic band structure calculation using 8 band  $k \cdot p$  method taking the  $\Gamma$  valley into consideration. The QD size effect on the fundamental transition energy is studied for optoelectronic device design.

## 2. Computational Methods

To simulate the interactions between atoms in our QD structure we use the VFF method with Keating potential [2], in which the strain energy,  $E_{strain}$  can be written as

$$E_{strain} = \frac{1}{2} \sum_{i(j)} \frac{3\alpha_{i-j}}{8d_{0,i-j}^2} \cdot (|\mathbf{x}_i - \mathbf{x}_j|^2 - d_{0,i-j}^2)^2 + \sum_{i(j,k)} \frac{3\beta_{j-i-k}}{8d_{0,i-j}d_{0,i-k}} \cdot [|\mathbf{x}_i - \mathbf{x}_j| \cdot |\mathbf{x}_i - \mathbf{x}_k| + \frac{1}{3}d_{0,i-j}d_{0,i-k}]^2 \quad (1)$$

The first summation runs over all atoms  $i$  and their four nearest neighbors  $j$ ; the second summation over all atoms  $i$  and their neighboring pairs  $j$  and  $k$ .  $\mathbf{x}_i$  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 its corresponding strain free lattice constant  $a_{0,i-j}$  as  $d_{0,i-j} = (\sqrt{3}/4)a_{0,i-j}$ .  $\alpha$  is the bond stretching force constant, and  $\beta$  is the bond bending force constant [2]. Values of  $\alpha$  and  $\beta$  are from [3]. To minimize the strain energy and attain system stability, we allow each atom to vibrate and move along the direction of force acting on it. The final location of each atom in the energy-minimized system is compared with its initial strain-free location, from which we can compute a 3D strain profile of the final system.

For the electronic band structure, we use the 8 band  $k \cdot p$  method at the  $\Gamma$  point. For GeSn, it is not reliable to use 6 band  $k \cdot p$  [4] as it fails to consider the interaction between the conduction band (CB) and valence band (VB). On the other hand 15 band  $k \cdot p$  [4] comes with the expense of introducing many fitting parameters, but is ideal to study the full extent of the Brillouin zone. For our work, the 8 band  $k \cdot p$  is accurate enough to study the subband energy dispersion curves near the  $\Gamma$  point of the [001] oriented GeSn/SiSn strained QDs. The Hamiltonian for the strained QD [5] can be simply written as  $H = H_k + V_F(z) + H_s$ , split into three matrices.  $H_k$  stands for the kinetic 8-band effective-mass Hamiltonian. This can incorporate the interaction between the CB and VB; and the spin-orbit (SO) coupling within the VB.  $V_F(z)$  accounts for the band offset effects in the strain-free condition, and  $H_s$  stands for the strain induced Hamiltonian. The  $8 \times 8$  expansion of the Hamiltonian matrices can be referred to our in previous work [5]. The material parameters used in the  $k \cdot p$  calculation are consistent with those used in our recent works [6, 7].

## 3. Results and Discussion

Our Ge<sub>0.5</sub>Sn<sub>0.5</sub>/Si<sub>0.5</sub>Sn<sub>0.5</sub> QD is pyramidal in shape with +z growth direction (Fig. 1); the base and wetting layer (two monolayers thick) are in the  $x$ - $y$  plane. The front view schematic of the QD system is shown in Fig. 2 (without the wetting layer for sake of simplicity). In the scope of our calculation, we vary the pyramidal QD's height ( $h$ ) from 6 to  $18 \times$  lattice constant ( $a$ ). Accordingly the entire system's height varies as  $3h$  and the length/width as  $4h$  (Fig. 2).

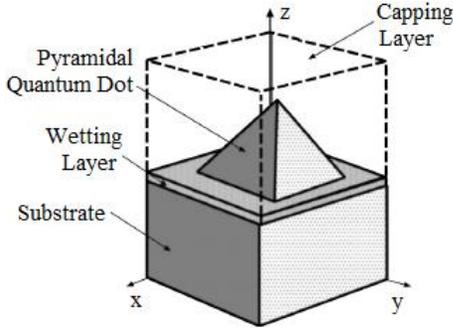


Fig. 1. 3D schematic of our pyramidal quantum dot

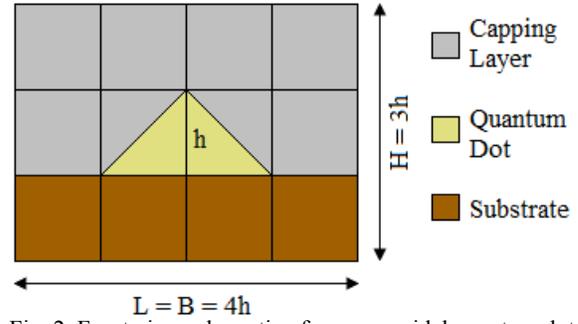


Fig. 2. Front view schematic of our pyramidal quantum dot

Fig. 3 shows the strain profile along [001] direction.  $\epsilon_{xx/yy}$  ( $\epsilon_{zz}$ ) increases (decreases) monotonically in the substrate and jumps to about -0.010 (+0.005) at the QD interface (wetting layer). Within the QD,  $\epsilon_{xx/yy}$  ( $\epsilon_{zz}$ ) increases (decreases) with a sudden jerk at the interface and changes sign (i.e. strain type). Finally in the capping layer both fall to zero. This result is consistent with [3, 7]. Fig. 4, 5, 6 shows the contour plot of  $\epsilon_{xx}$ ,  $\epsilon_{yy}$ ,  $\epsilon_{zz}$  in the (001) plane with  $z=1.5h$ . In Fig. 4 and 5, the yellowish and bluish zones experience compressive strain, while the reddish zones experience tensile strain; causing a strain gradient.

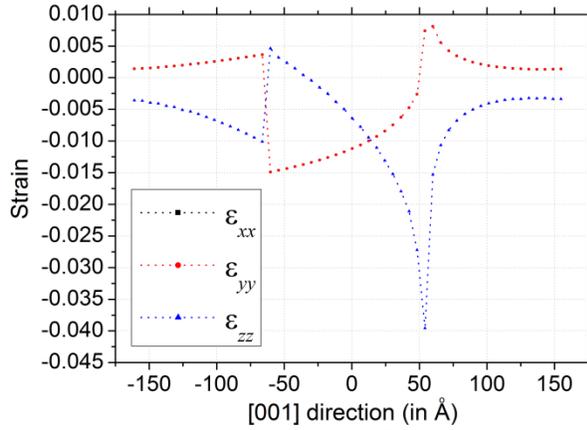


Fig. 3. Strain profile plot along [001] direction,  $x=y=0$

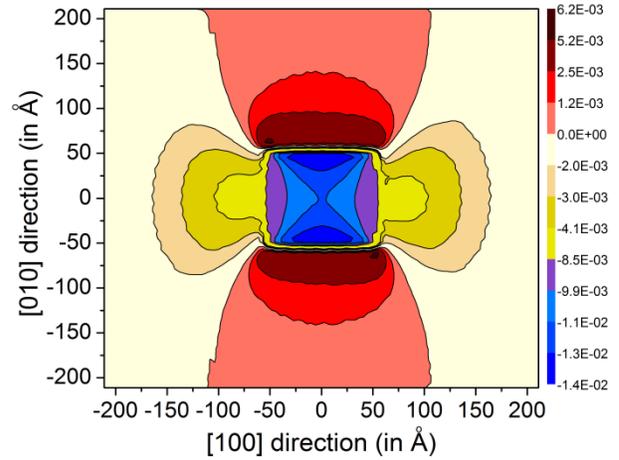


Fig. 4.  $\epsilon_{xx}$  contour plot in the (001) plane,  $z=1.5h$

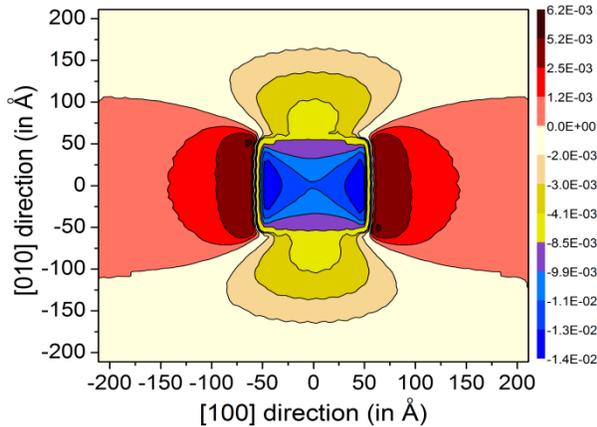


Fig. 5.  $\epsilon_{yy}$  contour plot in the (001) plane,  $z=1.5h$

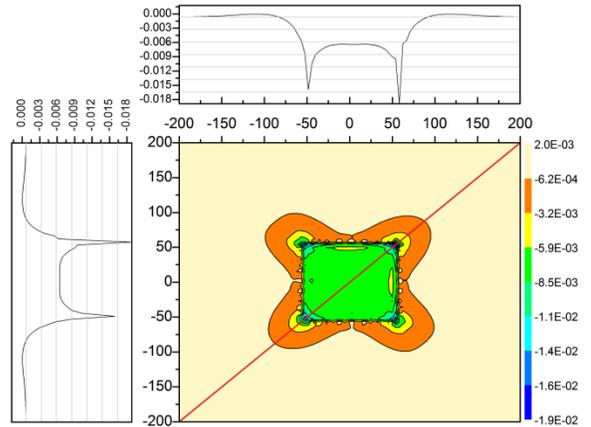


Fig. 6.  $\epsilon_{zz}$  contour plot in the (001) plane,  $z=1.5h$ ; & [110] direction

Fig. 4 and 5 can be easily correlated as  $\epsilon_{xx}$  along [010] is identical to  $\epsilon_{yy}$  along [100]; and  $\epsilon_{yy}$  in the [010] direction is identical to  $\epsilon_{xx}$  in the [100] direction. In Fig. 6, we see that there is very less compressive strain outside the QD, higher at the edges, highest at the corners, and intermediate within the QD. Here the skew red line shows the  $\epsilon_{zz}$  profile along [110] direction in (001) plane. It is noteworthy that Fig. 3 to 6 correspond to a QD height of  $h=18a$ .

Fig. 7 to 9 shows the energy profile at the  $\Gamma$  valley for varying QD height ( $h$ ) = 6, 12, 18  $\times a$ . The fundamental transition energy E1-H1 decreases as the QD size increases. This trend is plotted in Fig. 10, with additional data points:  $h = 6, 7, 8, 10, 11, 12, 15, 18 \times a$ , for which we have E1-H1 = 1079.27, 891.70, 667.96, 538.59, 521.54, 511.34, 451.57, 414.19 meV respectively. Curve fitting of the plot in Fig. 10 yields the relation,  $(E1 - H1) = [27.07499(h/a)^{-2} + 0.30776]$  eV, which is of course specific to our system in consideration, but nonetheless, helpful to estimate the bandgap of such quantum dot systems for designing optoelectronic devices.

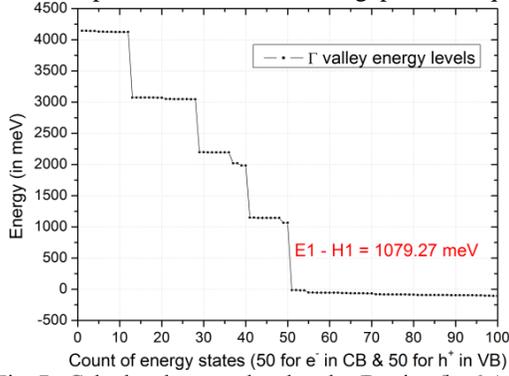


Fig. 7. Calculated energy level at the  $\Gamma$  point ( $h=6a$ )

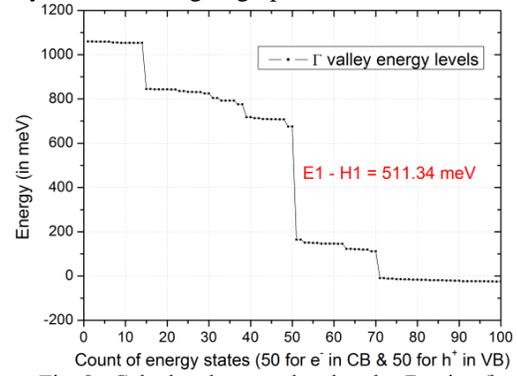


Fig. 8. Calculated energy level at the  $\Gamma$  point ( $h=12a$ )

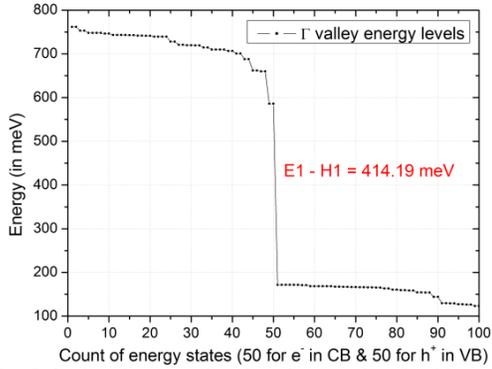


Fig. 9. Calculated energy level at the  $\Gamma$  point ( $h=18a$ )

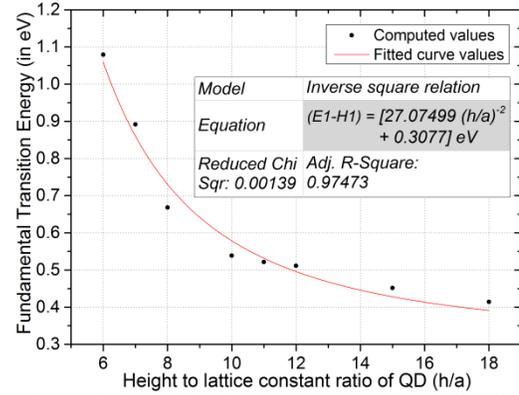


Fig. 10. Variation of E1-H1 energy vs. quantum dot size

## 5. Conclusion

We studied GeSn/SiSn QDs for their strain profile and electronic band structure using valence force field method and 8 band  $k \cdot p$  method respectively. The strain profile was studied in fair depth for the [001] direction and (001) plane, with distinct identification of zones of compressive and tensile strain. Thereafter, the size effect on the fundamental transition energy of the QD system was studied, which is an essential tuning factor in optoelectronic device designs. It is observed to predominantly vary inversely with the second power of QD height.

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