Electronic structure of Ge/Si self-assembled quantum dots

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Abstract

Pyramid and hut shapes of self-assembled Ge quantum dots over a range of the lateral size of less than 500 Å and dome structures beyond the lateral size of 1000 Å are typically observed. We have investigated the electronic properties of approximate models of the pyramid and hut structures by taking the profiles of strain components into account. To obtain the elastic strain distribution, a valence force field model is used. The electronic confined state energies for electrons and holes are then obtained by diagonalizing the resultant Hamiltonian matrix of the Schrödinger equation based on strain-modified potential. Theoretical results are compared with the transition energies observed by photoluminescence spectroscopy.

1. Introduction

The photoluminescence (PL) spectroscopy in self-assembled Ge/Si quantum dot (QD) structures have revealed the recombination peak distribution over an energy range of 0.75–0.9 eV [1,2]. The PL peaks in the same energy range have also been observed in $Si_{1-x}Ge_x$/Si quantum dots and $Si_{1-x}Ge_x$/Si quantum well structures containing high Ge contents [3]. Furthermore, the peaks in the annealed samples show shifts towards higher energies as the annealing temperature increases but are within the same energy range [2]. However, the relatively wide distribution of the peak positions has not been clarified, which may be mainly for lack of knowledge of the microscopic electronic structures. It seems that since the small structure is very sensitive to strain the simple application of an effective-mass approximation without detailed microscopic information such as strain profiles and strain-driven intermixing in the Ge/Si QDs leads to an overestimated (or underestimated) determination of the transition energies [4,5]. Recent experimental observations with techniques such as electron-dispersive x-ray (EDX) nanoanalysis, analysis of transmission electron diffraction (TED) patterns, and the image contrast method of transmission electron microscopy (TEM) have shown that there exist compositional interdiffusion between Ge QDs and Si layers [5-9]. Recently, this is further verified by a theoretical calculation of the electronic structure of self-assembled Ge quantum dots with a pyramidal shape [10]. In this work, we investigate the electronic properties of approximate models of the pyramid and hut structures since pyramid and hut shapes of self-assembled Ge quantum dots over a range of the lateral size of less

than 500 Å are typically observed and these are known to be more stable than other shapes such as "domes" [11,12,13].

2. Calculational approach

Figure 1 shows the models of pyramid and hut QDs grown on a wetting layer consisting of 3 monolayers (MLs) of Ge. They contain 76×76×26 and 86×66×27 conventional unit cells of diamond structure along x-, y-, and z-axes, respectively. Each model consists of about 1.2×10^6 atoms. The base width of the pyramid QD along the [100] direction and the height along the [001] direction consist of 60 and 5 conventional unit cells of Ge, respectively, and 70 and 5 cells for the hut QD. In addition, the roof of the hut QD corresponds to the edge length of 10 conventional unit cells.

To obtain the elastic strain distribution of a Ge QD structure including the wetting layer, a valence force field (VFF) model is useful [14]. In the model, the strain energy is given by

$$E = \frac{1}{2}\sum_i \sum_j^4 \frac{3\alpha_{ij}}{8d_{ij}^2}\left[(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 - d_{ij}^2\right]^2 + \sum_i \sum_j^4 \sum_{k=j+1}^4 \frac{3}{8d_{ij}d_{ik}}\left(\frac{\beta_{ij}+\beta_{ik}}{2}\right) \times\left[(\boldsymbol{r}_j - \boldsymbol{r}_i)\cdot(\boldsymbol{r}_k - \boldsymbol{r}_i) - d_{ij}d_{ik}\cos\theta_0\right]^2$$

where α and β describe bond stretching and bond bending forces, respectively, and θ_0 is the bond angle for bulk Si. The index i indicates the sum

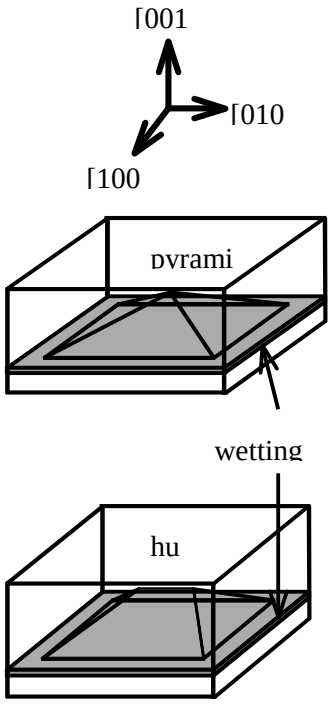

Fig. 1. Calculation models of pyramid and hut QDs and wetting layer.

over all atoms with nearest neighbors j and k and r_{ij} and d_{ij} are the strained and unstrained bond lengths, respectively. For the diamond structure $\cos\theta_0 = -1/3$. Details of the calculation method and parameters used have been reported elsewhere [10].

3. Results and discussion

The strain profiles of $\varepsilon_{xx}(=\varepsilon_{yy})$ and ε_{zz} along the growth direction through the pyramidal apex (a pyramid QD structure) and the roof center (a hut QD structure) obtained by elasticity energy minimization are shown in Figs. 2 (a) and (b). The positive strain values correspond to tensile strain and the negative ones to compressive strain. The in-plane strain ε_{xx} is almost zero from the

substrate bottom to near the interface of the wetting layer and substrate. However, ε_{zz} is considerably large due to the compressive and tensile strains inside the dot and in the Si layers, respectively. In particular, the strain is large near the Ge/Si interface regions. In addition, lateral

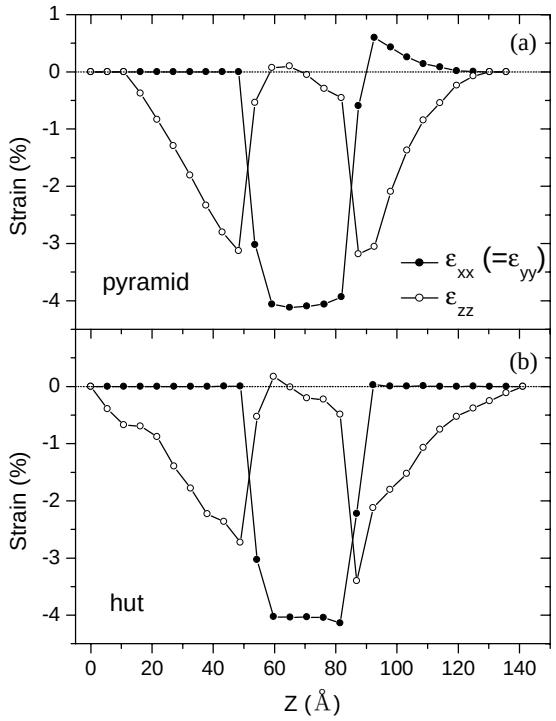

Fig. 2. Strain profiles along Z axis for pyramid (a) and hut (b) QD structures.

strain is maximum inside the Ge dot but the fractional volume change does not simply follow the Poisson ratio considering the change of ε_{zz}.

The band edge alignment between Si and Ge semiconductors without strain effects can be established according to the "model-solid theory" as shown in Fig. 3 [15]. The theory predicts band offsets in the conduction and valence bands of 0.34 and 0.767 eV, respectively. The absolute values of average valence band edges of Si and Ge of –7.03 and –6.35 eV are adopted from the literature [15].

Taking the band lineup and a three-dimensional distribution of the strain at every unit cell into account, the strain-modified energy band can be obtained. The results only along z-axis are shown in Fig. 4. The six degenerate electron states in the conduction band of Si near the interface

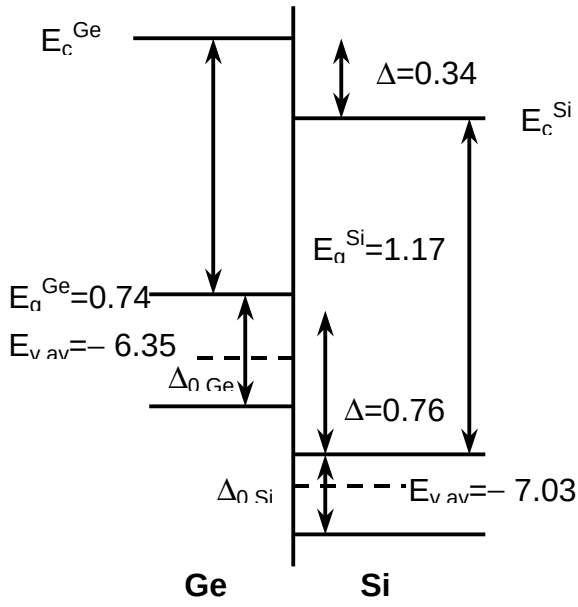

Fig. 3. Band lineup at the Ge/Si interface calculated by the model-solid theory. All values are in eV.

are split into twofold Δ_2 and fourfold Δ_4 states due to tensile strain. Contrary to the conduction band, the hole states of the valence band of Ge in the QDs are split due to compressive strain. Fig. 4 shows the three split states in the QDs.

The effective-mass approximation is used for the calculation of the three-dimensionally confined energy levels in the structure. For simplicity, the

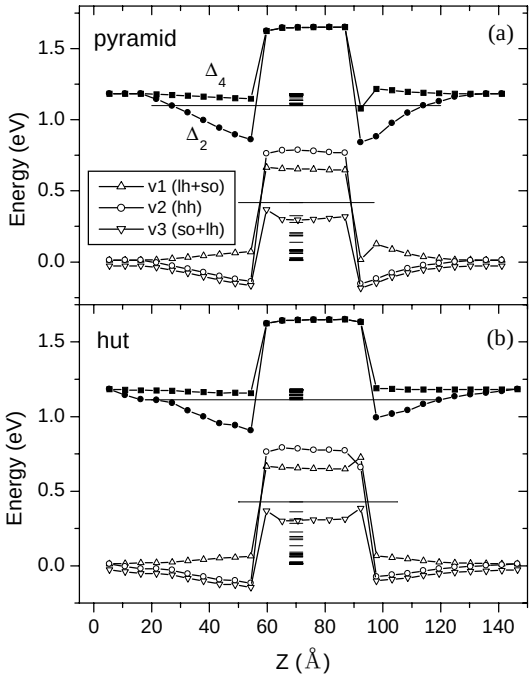

Fig. 4. Strain-modified band structures and confined energy levels for pyramid (a) and hut (b) structures.

decoupled conduction and valence bands are assumed. Furthermore, we considered that electrons are confined in the Δ_2 band of the Si barrier while holes are in the heavy hole band v_2. The single-band Schödinger equation,

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(\boldsymbol{r})\right]\phi(\boldsymbol{r}) = E\phi(\boldsymbol{r}) \qquad (2)$$

is then solved on the basis of consisting of 1331 plane waves where m^* is the effective mass, $\phi(\boldsymbol{r})$ is an envelope wave function and $V(\boldsymbol{r})$ is the three-dimensional confining potential. Here the confining potential is given as a function of position of each unit cell and is defined by the conduction (valence) band offset of the unit cell with respect to the Si conduction (valence) band edge. The resultant "strain" Hamiltonian matrix of the Schrödinger equation is diagonalized to obtain the eigenvalues. The effective masses for electron and heavy hole are $0.98m_0$ and $0.34\ m_0$, respectively. The long horizontal lines in Fig. 4 indicate the ground states while the short ones the higher levels. Some of higher levels are degenerate and thick levels represent continuous near Si band edges. Almost the same transition energy of 0.68 eV is obtained both for the pyramid and hut structures. That is, we may observe the same transition energies from the Ge QDs which are observed over the range of lateral size of smaller than 500 Å and have pyramid and hut shapes. More importantly, this transition energy is approximately more than 0.1 eV difference from the experimental values (i.e., 0.75–0.9 eV) and no PL peak measurement is reported near 0.68 eV. The results suggest that the Ge QDs can not formed only by pure Ge atoms, but they are, in fact, SiGe QDs.

It was recently recognized that significant interdiffusion between Si and Ge takes place from 20% up to 50% when Ge dots are capped with Si [8,9]. It is obvious that if the size of the assumed pure Ge dot increases the transition energy will be reduced due to reduced quantum confinement. Considering that the lateral size (about 340 Å) and the height (about 28 Å) adopted in the present model are smaller than the dots in the structures reported, we may not observe a larger transition energy than 0.68 eV. The reported transition energies of 0.75–0.9 eV observed from PL

measurements are inconsistent with the calculated results, which may be explained by the interdiffusion of Si into Ge dots during growth of the Si capping layer. Our calculation results thus suggest that self-assembled Ge QDs with a Si capping layer may not avoid such an intermixing phenomenon.

4. Conclusions

In conclusion, we have calculated the electronic structure of pyramid and hut shapes observed in self-assembled Ge QD structures and compared the transition energies with reported experimental results. From the calculational results we noticed that the transition energies of both shapes are almost same and significant interdiffusion between Ge and Si takes place. The calculational results also lead to a guideline to interpret PL spectroscopy in Ge or SiGe QD structures.

Acknowledgements

This work was supported by Korea Research Foundation grant (KRF-99-005-D00036).

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