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Strain-induced band profile of stacked InAs/GaAs Quantum Dots

Worasak Sukkabot *

Department of Physics, Faculty of Science, Ubon Ratchathani University, 85 Sathollmark Rd. Warinchamrab, Ubon Ratchathani, Thailand, 34190

(*Corresponding author's e-mail: w.sukkabot@gmail.com)

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Abstract

We have calculated the strain distribution and band profile in triply stacked InAs/GaAs quantum dots (QDs) with the dot spacing 0.0-6.0 nm. We have used the continuum elasticity theory for the strain distribution and the eight-band k.p theory for the band structure. We report the use of the k.p method to calculate the band structure with and without including the effects of strain. The calculated results show the importance of strain effect on the confinement potential of the band structure for triply stacked InAs/GaAs quantum dots (QDs).

Keywords: Stacked quantum dots, strain distribution and k.p method

Introduction

Research and development in semiconductor has seen progressive reduction in dimension, from bulk material to quantum well, then to quantum wire, and ultimately to quantum dot. Thus, the three-dimensional carrier confinement property can significantly lead to the superior characteristics of atom-like density-of-states (DOS), large exciton binding energies and enhanced oscillator strength in quantum dots. The quantum dots (QDs) can be the candidates in transistors, solar cells, LEDs, and diode lasers. They can be also represented as the agents for medical imaging and as possible qubits in quantum computing. Electronic structure and optical properties of semiconductor quantum dots have been intensively explored for more than two decades from the physical and technological interests to the zero-dimensional confined systems [1]. For example, the emission energy and carrier relaxation process in the 2-10-layer stacked InAs QDs with few-nm spacing have been studied in detail [2]. Recently vertically stacked InAs/GaAs quantum dots (QDs) have been investigated for the application to the quantum dot lasers and quantum computers [3]. Kita et al. [4, 5] experimentally demonstrated that the optical polarization can be controlled in the columnar InAs/GaAs quantum dots, in which the self-assembled QDs are vertically stacked with no inter-dot barrier layers. Saito et al. [3, 6] calculated the strain distribution and electronic structures in the stacked InAs/GaAs QDs with the dot spacing 0-6 nm; based on the elastic continuum theory and eight-band k.p theory. They also theoretically studied the optical polarization in columnar InAs/GaAs quantum dots. Janusz Andrzejewski et al. [7] presented the eight-band k.p calculations of the electronic and polarization properties for the columnar $In_zGa_{1-z}As$ quantum dots with high aspect ratio embedded in an $In_xGa_{1-x}As/GaAs$ quantum well. However, the previous studies have not investigated the dependence of dot spacing on the strain tensors and also the strain-induced band profile of the stacked quantum dots. The fundamental knowledge of this work can be implemented further to study the control of the polarization in stacked quantum dots that can be highly beneficial in some optoelectronic applications. According to the previous research, the stacked InAs/GaAs quantum dots with 0.0 nm spacing, generally called columnar QDs (CQDs) are significantly promising candidates for amplifier applications.

In order to understand the physical properties of the triply stacked quantum dots, theoretical calculations of the electronic structures based on the realistic strain distribution are essential. In this study, we calculate the strain distribution in the stacked InAs/GaAs quantum dots with the dot spacing in the range from 0 nm to 6 nm based on the continuum elasticity (CE) theory. The confinement potentials are numerically evaluated by means of the eight-band strain-dependent k.p theory. Finally, the band alignments are numerically evaluated with and without taking account into the strain field.

Theory

Strain Distribution

The atomic positions inside and around the quantum dot can be described in terms of the supercell of the Face-centered cubic structure. Due to the lattice mismatch between quantum dot and surrounding material, the atomic positions can change and the strain field also takes place in this structure. The continuum elasticity (CE) is determined to study this purpose. The total strain energy in the CE model is given by [3, 8, 9]:

$$U_{CE} = \frac{1}{2}\sum_{i,j,k,l} C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}$$

For a given structure, U_{CE} can be minimized by implementing the finite difference method for the strains $\varepsilon_{ij} = \left(\frac{du_i}{dx_j} + \frac{du_j}{dx_i}\right)/2$, where u is the displacement vector field. The elastic moduli C_{ijkl} are represented by the parameters C_{11}, C_{12} and C_{44} for cubic crystals. Table I shows the material parameters [10] used for the calculations.

Eight-band strain-dependent k.p method

The influence of the strain profiles on the electronic structure of quantum dots has been previously investigated by implementing the strain-modified band offsets [11]. The strain-modified confinement potentials can be calculated by means of the eight-band strain-dependent k.p Hamiltonian, $H_k + H_s$, where H_k is the kinetic Hamiltonian and H_s is the strained Hamiltonian. The kinetic part of the total Hamiltonian is given by:

$$\begin{bmatrix}
A & 0 & V^* & 0 & \sqrt{3}V & -\sqrt{2}U & -U & \sqrt{2}V^* \\
0 & A & -\sqrt{2}U & -\sqrt{3}V^* & 0 & -V & \sqrt{2}V & U \\
V & -\sqrt{2}U & -P+Q & -S^* & R & 0 & \sqrt{\frac{3}{2}}S & -\sqrt{2}Q \\
0 & -\sqrt{3}V & -S & -P+Q & 0 & R & -\sqrt{2}R & \frac{1}{\sqrt{2}}S \\
\sqrt{3}V^* & 0 & R^* & 0 & -P+Q & S^* & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R^* \\
-\sqrt{2}U & -V^* & 0 & R^* & S & -P+Q & \sqrt{2}Q & \sqrt{\frac{3}{2}}S^* \\
-U & \sqrt{2}V^* & \sqrt{\frac{3}{2}}S^* & -\sqrt{2}R^* & \frac{1}{\sqrt{2}}S & \sqrt{2}Q & -P+\Delta & 0 \\
\sqrt{2}V & U & -\sqrt{2}Q & \frac{1}{\sqrt{2}}S^* & \sqrt{2}R & \sqrt{\frac{3}{2}}S & 0 & -P+\Delta
\end{bmatrix}$$

Where

$$A = E_c - \frac{\hbar^2}{2m_0}(k_x^2 + k_y^2 + k_z^2)$$

$$B = E_c - \gamma_1 \frac{\hbar^2}{2m_0}(k_x^2 + k_y^2 + k_z^2)$$

$$Q = -\gamma_2 \frac{\hbar^2}{2m_0}(k_x^2 + k_y^2 + k_z^2)$$

$$R = \sqrt{3}\frac{\hbar^2}{2m_0}[\gamma_2(k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y]$$

$$S = -\sqrt{3}\gamma_3 \frac{\hbar^2}{2m_0} k_z (k_x - ik_y)$$

$$U = \frac{-i}{\sqrt{3}} P_0 k_z$$

$$V = \frac{-i}{\sqrt{6}} P_0 (k_x - ik_y)$$

P_0 is the coupling between the conduction and valence bands, E_c and E_v are the unstrained conduction and valence band energy, respectively, and Δ is the spin-orbit splitting. The $\gamma_{i=1,2,3}$ are the modified Luttinger parameters defined in terms of the usual Luttinger parameters $\gamma^L_{i=1,2,3}$:

$$\gamma_1 = \gamma_1^L - \frac{E_p}{3E_g + \Delta}$$
$$\gamma_2 = \gamma_2^L - \frac{1}{2}\frac{E_p}{3E_g + \Delta}$$
$$\gamma_3 = \gamma_3^L - \frac{1}{2}\frac{E_p}{3E_g + \Delta}$$

$E_g = E_c - E_v$ is the energy gap and $E_p = 2m_0P_0^2/\hbar^2$. The strained part of the total Hamiltonian is also given by:

$$\begin{bmatrix}
a_c e & 0 & -v^* & 0 & -\sqrt{3}v & \sqrt{2}u & u & -\sqrt{2}v^* \\
0 & a_c e & \sqrt{2}u & \sqrt{3}v^* & 0 & v & -\sqrt{2}v & -u \\
-v & \sqrt{2}u & -p+q & -s^* & r & 0 & \sqrt{\frac{3}{2}}s & -\sqrt{2}q \\
0 & \sqrt{3}v & -s & -p+q & 0 & r & -\sqrt{2}r & \frac{1}{\sqrt{2}}s \\
-\sqrt{3}v^* & 0 & r^* & 0 & -p+q & s^* & \frac{1}{\sqrt{2}}s^* & \sqrt{2}r^* \\
\sqrt{2}u & v^* & 0 & r^* & s & -p+q & \sqrt{2}q & \sqrt{\frac{3}{2}}s^* \\
u & -\sqrt{2}v^* & \sqrt{\frac{3}{2}}s^* & -\sqrt{2}r^* & \frac{1}{\sqrt{2}}s & \sqrt{2}q & -p & 0 \\
-\sqrt{2}v & u & -\sqrt{2}q & \frac{1}{\sqrt{2}}s^* & \sqrt{2}r & \sqrt{\frac{3}{2}}s & 0 & -p
\end{bmatrix}$$

Where

$$e = e_{xx} + e_{yy} + e_{zz}$$
$$p = a_v(e_{xx} + e_{yy} + e_{zz})$$
$$q = b[e_{zz} - \frac{1}{2}(e_{xx} + e_{yy})]$$
$$r = \frac{\sqrt{3}}{2}b(e_{xx-e_{yy}}) - ide_{xy}$$
$$s = -d(e_{xz} - ie_{yz})$$
$$u = \frac{-i}{\sqrt{3}}P_0\sum_j e_{zj}k_j$$
$$v = \frac{-i}{\sqrt{6}}P_0\sum_j (e_{xj} - ie_{yj})k_j$$

e_{ij} is the strain tensor, b and d are the shear deformation potentials. a_v is the hydrostatic valence band deformation potential and a_c is the conduction-band deformation potential. Table II [11] lists the material parameters which are used to calculate the strain-induced confinement potentials.

After the total Hamiltonian ($H_k + H_s$) matrix elements are constructed, the matrix can be diagonalized by using the powerful eigenvalue solver called EISPACK library [12]. Finally, strain-induced band alignments are achieved.

Results and discussion

To investigate the influence of the strain field on the stacked InAs/GaAs quantum dots, recently there are various layers of the InAs dots (1-9) that have been studied in theory and experiment. In this work, the stacked quantum dot structures are modeled by triply vertically stacked InAs quantum dots embedded in GaAs surrounding material corresponding to the accessible range in the theoretical and experimental data. The growth direction is mainly aligned along the z axis. Each InAs quantum dot has a truncated pyramidal shape because of the realistic shape mostly fabricated in the experiments. The dot height is 3.0 nm and the length of the square base is 15.0 nm. The dot spacing varies from 0.0 to 6.0 nm. The cross-sectional view of the triply stacked quantum dot structures is depicted in Figure 1. The strain distribution in the stacked quantum dots can be evaluated using a finite difference method based on the continuum elasticity theory. This method has fruitfully implemented to single pyramidal quantum dots in the previous studies [13, 14].

To analyze the band profiles of the triply vertically stacked InAs/GaAs quantum dots as described in the section of Eight-band strain-dependent k.p method, the calculations of the hydrostatic and biaxial strains are mainly required. The hydrostatic $\varepsilon_H = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$ and biaxial $\varepsilon_B = \varepsilon_{zz} - (\varepsilon_{xx} + \varepsilon_{yy})/2$ strains can determine the change of band confinement potential. The hydrostatic strains defined in the on-site diagonal term of H_s merely shift the energy levels of conduction and valence bands. While the biaxial strains defined in both of the on-site and off-site diagonal term of H_s intend to remove the degeneracy in the valence bands. Therefore, we numerically investigate the effect of the dot spacing on the hydrostatic and biaxial strains. Figure 2 illustrates the physical distribution of the hydrostatic and biaxial strain in the triply stacked InAs/GaAs quantum dots as a function of the dot spacings. The strain distribution along the z-axis (the line through the quantum dot center) is plotted. In the GaAs barrier regions, the hydrostatic strain is almost zero. In the quantum dot regions, the hydrostatic strain is approximately -0.08. The hydrostatic strain is mostly confined in the dots. The calculations demonstrate that there is compressive ($\varepsilon_H < 0$) strain inside the quantum dot regions because GaAs surrounding material compresses the InAs dots. For 0.0 nm spacing, the biaxial strain is even smaller and eventually becomes negative in the middle of the stacked quantum dots. As increasing the spacing of the stack triply quantum dots, the biaxial strain in the quantum dot regions positively increases. This is due to the condition that the vertical lattice constant of InAs mis-match that of the side GaAs when the barriers are inserted to the triply stacked quantum dots. In the barriers, the biaxial strain is negative. With increasing the spacing, the biaxial strain gradually enhances.

After understanding the physical behaviors of the strain distribution, the strain tensors and deformation potentials can be numerically used to calculate the strain-induced confinement potentials for the triply stacked InAs/GaAs quantum dots. Based on the eight-band strain-dependent k.p method as described above, we compute the influences of the strain and dot spacing on the conduction band edge, the heavy-hole band edge, light-hole band edge and spin-orbit band edge as shown in Figure 3. In this model, we use the valence band offset between InAs/GaAs junction as +0.25 eV [9]. The confinement potentials are calculated with and without taking into account the strain effect. We find that the strain distribution can essentially modify the band profile in the stacked quantum dots. The numerical results demonstrate that the biaxial strain induces a different shift of degeneracy between the heavy hole and the

light hole band as compared to the unstrained band profile which are equated in the strained Hamiltonian (H_s) defined as the diagonal q term. In the conduction band (CB) the strain principally yields the rising confinement potentials in the dots, while confinement potentials in the barrier indifferently change. The enhancement and invariant of the conduction band (CB) can be caused from the hydrostatic strain (ε_H). In the heavy hole band (HH), the strain mainly elevates the confinement potentials in the dots, interface and the inter-dots, while ones in the barriers far way from dots unimportantly modify. In the light-hole (LH) and spin-orbit (SO) band, the strain mainly lowers the confinement potentials in the inter-dots and the interfaces, while ones in the dots and the barriers far way from dots insignificantly alter. From the strained-induced band profiles of the triply stacked quantum dots, the numerical data demonstrates that the energies of the confining electron and hole states mainly rise into the higher energies as compared to the unstrained band alignments. In term of the dot spacing, there is no alteration in the unstrained band profiles, while the strained ones are principally modified. The strained band alignments of both conduction and valence band in the dots unconcernedly change. However, the strained band profiles in the inter-dot regions modify. As increasing the dot spacing, strained potential confinements in the inter-dot zones become smooth and are close to unstrained ones because the coupling of the stacked quantum dots progressively reduces.

Conclusion

We have systematically discussed the strain distributions of triply vertically stacked InAs/GaAs quantum dots with the dot spacing ranging from 0.0 nm to 6.0 nm. First, based on the finite difference method, we calculate the strain distribution by means of the elastic continuum theory. Secondly, the strained-modified band edges are also calculated in the framework of the eight-band strain-dependent k.p method. The calculations demonstrate that there is compressive ($\varepsilon_H < 0$) strain in the quantum dot region. With increasing the dot spacing of the stack triply quantum dots, the biaxial strain in both of the quantum dot regions and barriers positively raises. The hydrostatic and biaxial strains are used to judge the change of band profiles. The hydrostatic strains shift the energy levels of conduction and valence bands, while the biaxial strains eliminate the degenerate valence bands. Finally, the strain distribution and dot spacings have the significant effect in modifying the band structure of stacked triply InAs/GaAs quantum dots.

Acknowledgements

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Table I. Material parameters for the calculations.

	C_{11}(GPa)	C_{12}(GPa)	C_{44}(GPa)	e_{14}(C.m^{-2})	ε
InAs	83.3	45.3	39.6	-0.115	14.6
GaAs	118.8	53.8	59.4	-0.230	13.18

Table II. Material parameters.

Parameters	InAs	GaAs
γ_1^L	19.67	6.85
γ_2^L	8.37	2.1
γ_3^L	9.29	2.9
E_g(eV)	0.418	1.519
Δ(eV)	0.38	0.33
E_p(eV)	22.2	25.7
a_c(eV)	-6.66	-8.6
a_v(eV)	0.66	-9.3
b(eV)	-1.8	0.7
d(eV)	-3.6	-2.0

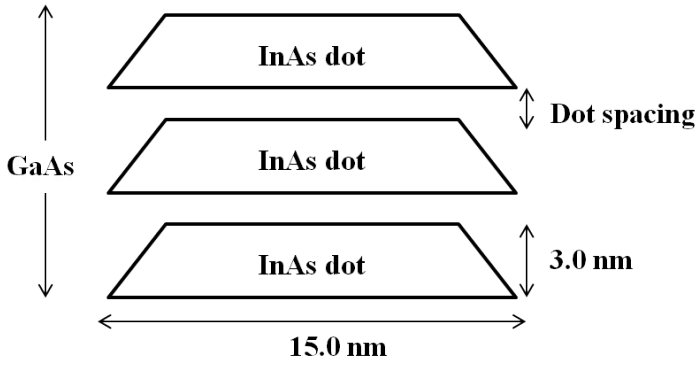

Figure 1 The cross-sectional picture of the triply stacked InAs/GaAs quantum dots.

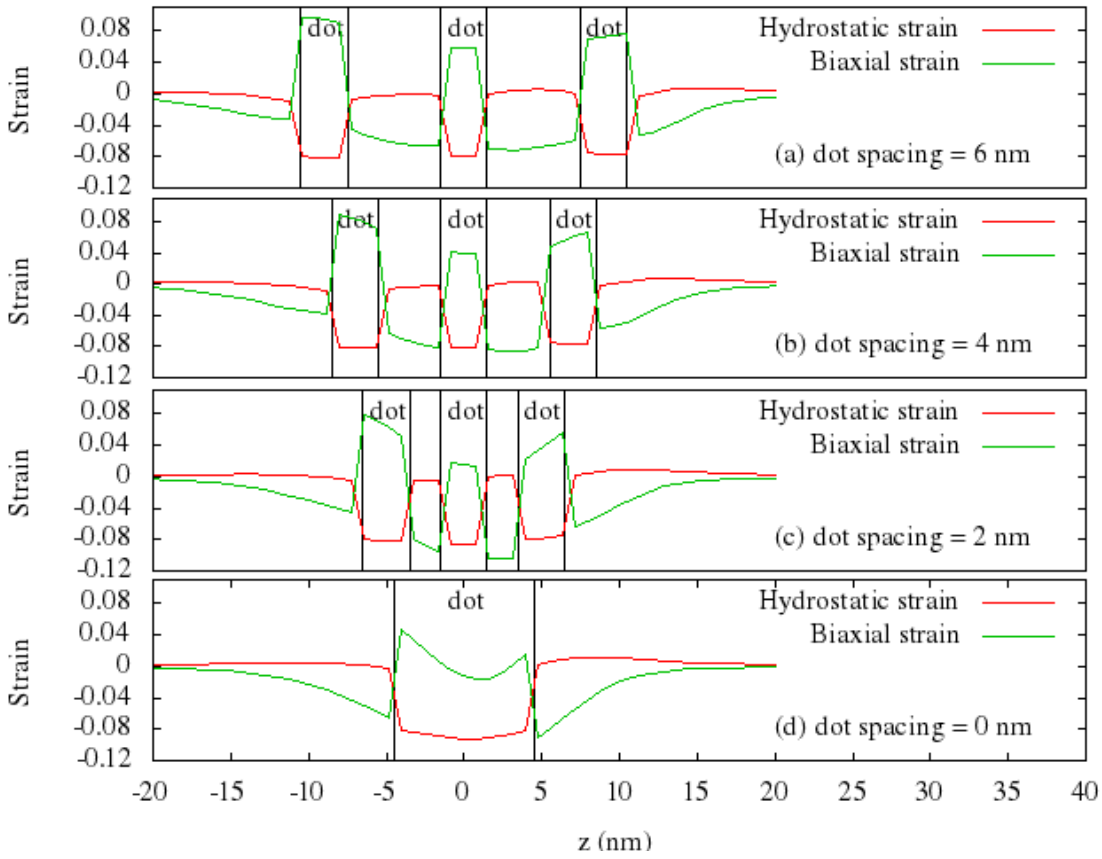

Figure 2 Strain distributions in the triply stacked InAs/GaAs quantum dots for the dot spacing; (a) 6 nm, (b) 4 nm, (c) 2 nm and (d) 0 nm.

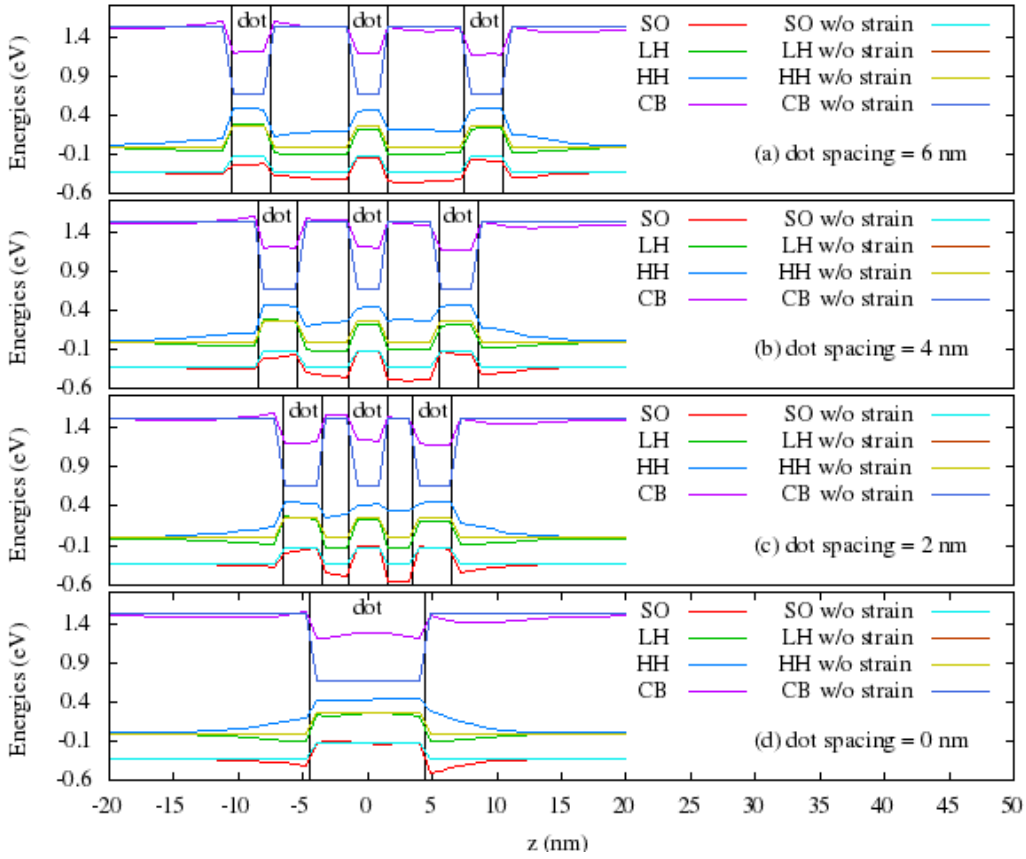

Figure 3 Strain-induced band profiles of the triply stacked InAs/GaAs quantum dots along the z direction for the dot spacing; (a) 6 nm, (b) 4 nm, (c) 2 nm and (d) 0 nm.