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Strain-Induced Band Profile of Stacked InAs/GaAs Quantum Dots

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Abstract

The strain distribution and band profile in triply stacked InAs/GaAs quantum dots with dot spacing of 0.0 - 6.0 nm was calculated. The continuum elasticity theory for strain distribution and 8-band k.p theory for band structure was used. The use of the k.p method to calculate band structure with and without including the effects of strain is reported. The calculated results show the importance of strain effect on the confinement potential of the band structure for triply stacked InAs/GaAs quantum dots.

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

Introduction

Research and development in the field of semiconductors has seen progressive reduction in dimension, from bulk material to quantum well, then to quantum wire, and ultimately to quantum dot. Thus, 3-dimensional carrier confinement property can significantly lead to superior characteristics of atom-like density-of-states (DOS), large exciton binding energies, and enhanced oscillator strength in quantum dots. The quantum dots can be candidates in transistors, solar cells, LEDs, and diode lasers. They can be also be used as agents in medical imaging and as possible qubits in quantum computing. The electronic structure and optical properties of semiconductor quantum dots have been intensively explored for more than 2 decades, from physical and technological interests to zero-dimensional confined systems [1]. For example, the emission energy and carrier relaxation process in the 2-10-layer stacked InAs quantum dots with few-nm spacing has been studied in detail [2]. Recently, vertically stacked InAs/GaAs quantum dots have been investigated for their application to quantum dot lasers and quantum computers [3]. Kita *et al*. [4,5] experimentally demonstrated that optical polarization can be controlled in the columnar InAs/GaAs quantum dots, in which the self-assembled quantum dots are vertically stacked with no inter-dot barrier layers. Saito *et al*. [3,6] calculated strain distribution and electronic structures in stacked InAs/GaAs quantum dots with dot spacing of 0 - 6 nm, based on the elastic continuum theory and 8-band k.p theory. They also theoretically studied the optical polarization in columnar InAs/GaAs quantum dots. Andrzejewski *et al*. [7] presented 8-band k.p calculations of the electronic and polarization properties for columnar $In_zGa_{1-z}As$ quantum dots with a high aspect ratio embedded in an $In_xGa_{1-x}As/GaAs$ quantum well. However, these previous studies did not investigate the dependence of dot spacing on the strain tensors or 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 polarization in stacked quantum dots, which could be highly beneficial in some optoelectronic applications. According to the previous research, stacked InAs/GaAs quantum dots with 0.0 nm spacing, generally called columnar quantum dots (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 realistic strain distribution are essential. In this study, the strain distribution in the stacked InAs/GaAs quantum dots with dot spacing in the range from 0 nm to 6

nm are calculated based on the continuum elasticity (CE) theory. The confinement potentials are numerically evaluated by means of the 8-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 the quantum dot and the surrounding material, the atomic positions can change, and the strain field takes place in this structure. Continuum elasticity (CE) is determined to study this purpose. The total strain energy in the CE model is given by [3,8,9];

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

For a given structure, U_{CE} can be minimized by implementing the finite difference method for the;

$$\text{strains } \varepsilon_{ij} = \left(\frac{du_i}{dx_j} + \frac{du_j}{dx_i}\right)/2, \tag{2}$$

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 1** shows the material parameters [10] used for the calculations.

Table 1 Material parameters for 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

8-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 strain-modified band offsets [11]. The strain-modified confinement potentials can be calculated by means of the 8-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;

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

where

$$\begin{aligned}
A &= E_c - \frac{\hbar^2}{2m_0}(k_x^2 + k_y^2 + k_z^2) \\
B &= E_c - \gamma_1 \frac{\hbar^2}{2m_0}(k_x^2 + k_y^2 + k_z^2) \\
Q &= -\gamma_2 \frac{\hbar^2}{2m_0}(k_x^2 + k_y^2 + k_z^2) \\
R &= \sqrt{3}\frac{\hbar^2}{2m_0}[\gamma_2(k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y] \\
S &= -\sqrt{3}\gamma_3 \frac{\hbar^2}{2m_0} k_z (k_x - ik_y) \\
U &= \frac{-i}{\sqrt{3}} P_0 k_z \\
V &= \frac{-i}{\sqrt{6}} P_0 (k_x - ik_y)
\end{aligned} \quad (4)$$

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

$$\gamma_1 = \gamma_1^L - \frac{E_p}{3E_g + \Delta}$$
$$\gamma_2 = \gamma_2^L - \frac{1}{2}\frac{E_p}{3E_g + \Delta} \quad (5)$$
$$\gamma_3 = \gamma_3^L - \frac{1}{2}\frac{E_p}{3E_g + \Delta}$$

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

$$\begin{bmatrix}
a_c e & 0 & -v^* & 0 & -\sqrt{3}v & \sqrt{2}u & u & -\sqrt{2}v^* \\
0 & a_c e & \sqrt{2}u & \sqrt{3}v^* & 0 & v & -\sqrt{2}v & -u \\
-v & \sqrt{2}u & -p+q & -s^* & r & 0 & \sqrt{\frac{3}{2}}s & -\sqrt{2}q \\
0 & \sqrt{3}v & -s & -p+q & 0 & r & -\sqrt{2}r & \frac{1}{\sqrt{2}}s \\
-\sqrt{3}v^* & 0 & r^* & 0 & -p+q & s^* & \frac{1}{\sqrt{2}}s^* & \sqrt{2}r^* \\
\sqrt{2}u & v^* & 0 & r^* & s & -p+q & \sqrt{2}q & \sqrt{\frac{3}{2}}s^* \\
u & -\sqrt{2}v^* & \sqrt{\frac{3}{2}}s^* & -\sqrt{2}r^* & \frac{1}{\sqrt{2}}s & \sqrt{2}q & -p & 0 \\
-\sqrt{2}v & u & -\sqrt{2}q & \frac{1}{\sqrt{2}}s^* & \sqrt{2}r & \sqrt{\frac{3}{2}}s & 0 & -p
\end{bmatrix} \quad (6)$$

where

$$e = e_{xx} + e_{yy} + e_{zz}$$
$$p = a_v(e_{xx} + e_{yy} + e_{zz})$$
$$q = b[e_{zz} - \frac{1}{2}(e_{xx} + e_{yy})]$$
$$r = \frac{\sqrt{3}}{2}b(e_{xx} - e_{yy}) - ide_{xy} \quad (7)$$
$$s = -d(e_{xz} - ie_{yz})$$
$$u = \frac{-i}{\sqrt{3}}P_0\sum_j e_{zj}k_j$$
$$v = \frac{-i}{\sqrt{6}}P_0\sum_j (e_{xj} - ie_{yj})k_j$$

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 2** [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.

Table 2 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

Results and discussion

In investigating the influence of the strain field on the stacked InAs/GaAs quantum dots, there are various layers of the InAs dots (1 - 9) that have been studied recently in theory and by experiment that should be considered. 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 this is the standard 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 been fruitfully implemented in previous studies of single pyramidal quantum dots [13,14].

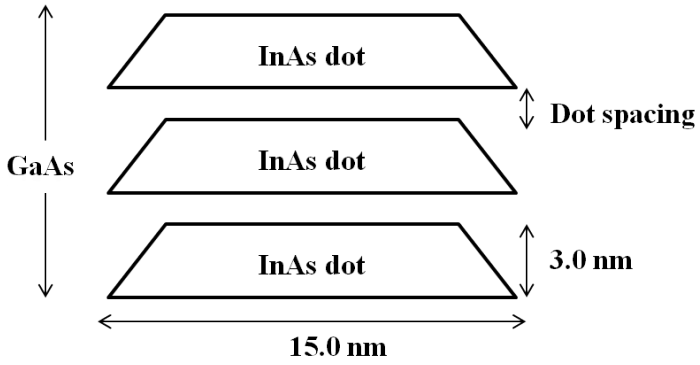

Figure 1 Cross-section of triply stacked InAs/GaAs quantum dots.

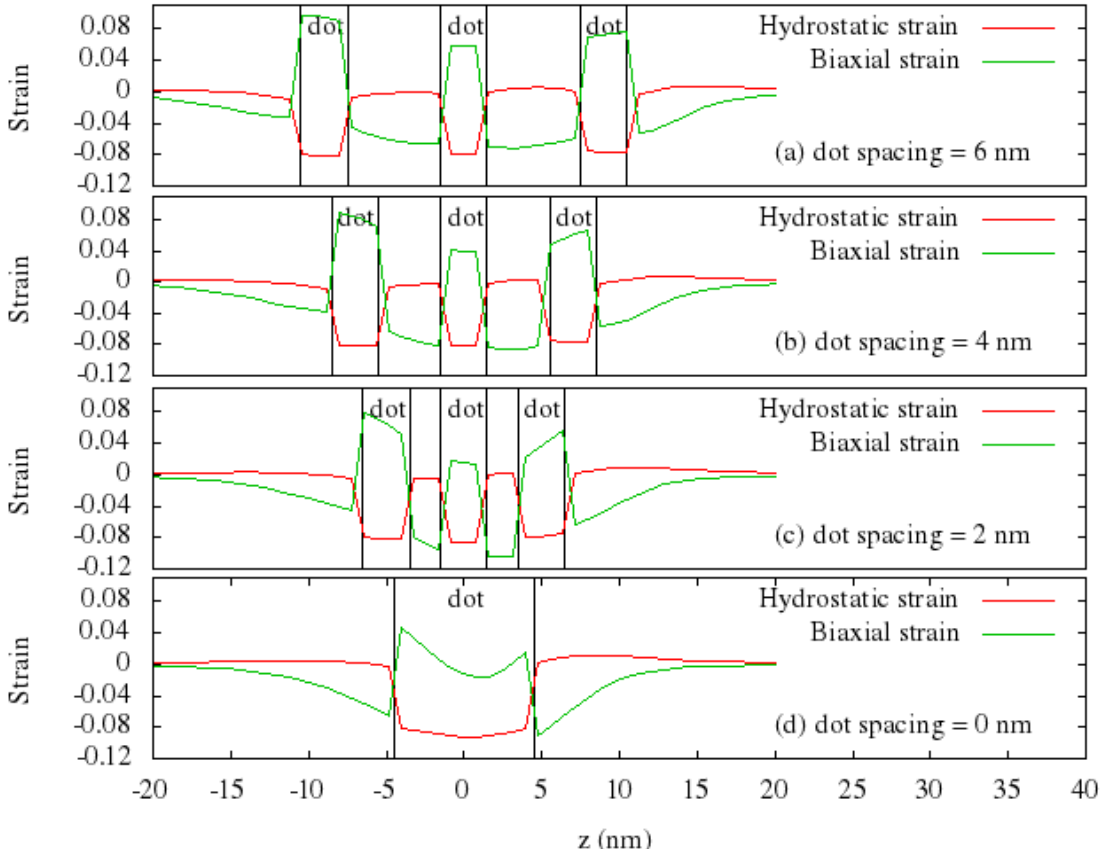

Figure 2 Strain distributions in triply stacked InAs/GaAs quantum dots with dot spacing of (a) 6 nm, (b) 4 nm, (c) 2 nm and (d) 0 nm.

To analyze the band profiles of the triply vertically stacked InAs/GaAs quantum dots as described by the section of 8-band strain-dependent k.p method, calculations of the hydrostatic and biaxial strains are required. The hydrostatic $\varepsilon_{\mathrm{H}} = \varepsilon_{\mathrm{xx}} + \varepsilon_{\mathrm{yy}} + \varepsilon_{\mathrm{zz}}$ and biaxial $\varepsilon_{\mathrm{B}} = \varepsilon_{\mathrm{zz}} - (\varepsilon_{\mathrm{xx}} + \varepsilon_{\mathrm{yy}})/2$ strains can determine the change of band confinement potential. The hydrostatic strains defined in the on-site diagonal term of $\mathrm{H_s}$ 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 $\mathrm{H_s}$ intend to remove the degeneracy in the valence bands. Therefore, the effect of dot spacing on the hydrostatic and biaxial strains is numerically investigated. **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 a compressive ($\varepsilon_{\mathrm{H}} < 0$) strain inside the quantum dot regions, because the 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. Increasing the spacing of the stack triply quantum dots results in the biaxial strain in the quantum dot regions positively increasing. This is due to the condition that the vertical lattice constant of InAs mismatch 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 an increase of the spacing, the biaxial strain is gradually enhanced.

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 8-band strain-dependent k.p method as described above, 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 are calculated, as shown in **Figure 3**. In this model, the valence band offset between InAs/GaAs junction as +0.25 eV [9] is used. The confinement potentials are calculated with and without taking into account the strain effect. It is found 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 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 can be caused by 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 away from the dots are minimally modified. 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 away from dots are insignificantly altered. 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 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 the conduction and valence bands in the dots unconcernedly change. However, the strained band profiles in the inter-dot regions modify. When 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.

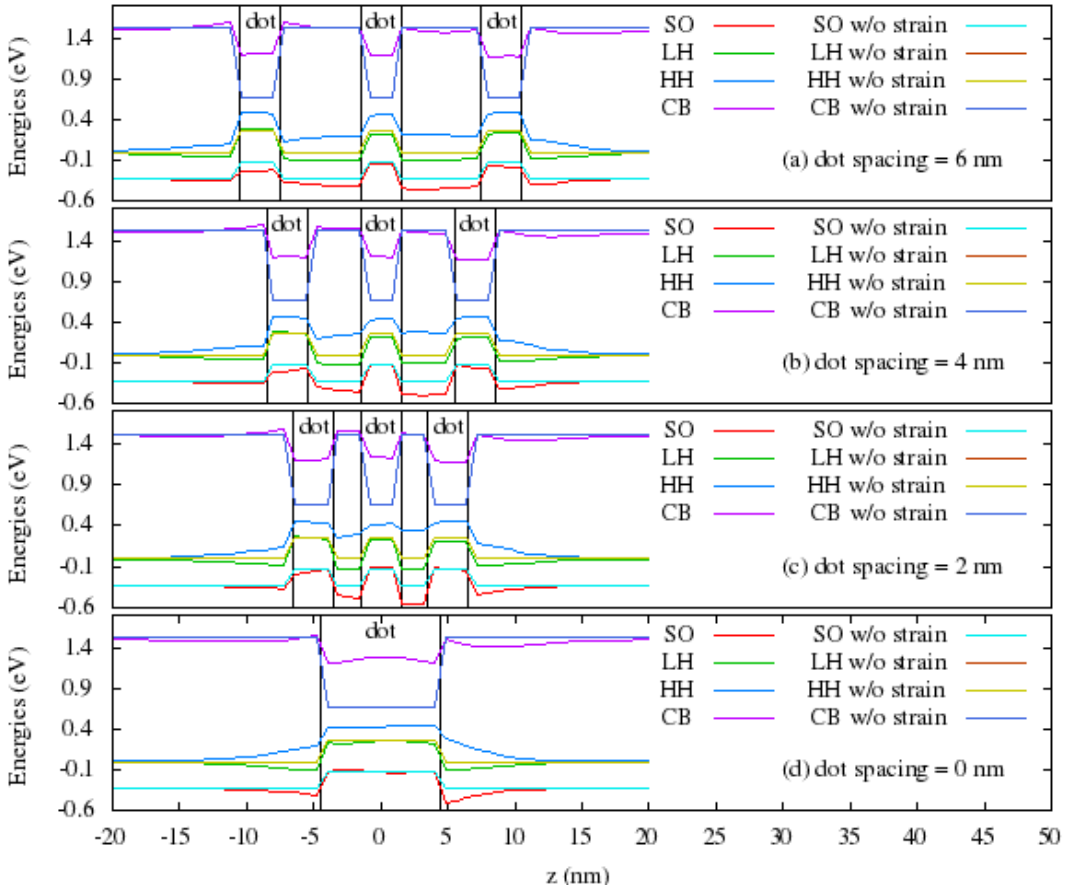

Figure 3 Strain-induced band profiles of triply stacked InAs/GaAs quantum dots along z direction with dot spacing of (a) 6 nm, (b) 4 nm, (c) 2 nm and (d) 0 nm.

Conclusions

The strain distributions of triply vertically stacked InAs/GaAs quantum dots with dot spacing ranging from 0.0 nm to 6.0 nm have been systematically discussed. First, based on the finite difference method, the strain distribution by means of the elastic continuum theory was calculated. Secondly, the strained-modified band edges were also calculated in the framework of the 8-band strain-dependent k.p method. The calculations demonstrate that there is a compressive ($\varepsilon_{\mathrm{H}} < 0$) strain in the quantum dot region. With an increase in the dot spacing of the triply stacked 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 the conduction and valence bands while the biaxial strains eliminate the degenerate valence bands. Finally, the strain distribution and dot spacings have a significant effect in modifying the band structure of triply stacked InAs/GaAs quantum dots.

Acknowledgements

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