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Research Article

Effect of the strain distribution and piezoelectricity on Quantum Dots: k.p method

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Abstract

This paper presents the calculations of the electronic structure and strain distribution for self-organized InAs/GaAs quantum dots. The strain calculations are based on the continuum elastic theory. The piezoelectric potential is calculated by solving the 3D Poisson's equation. The electron and hole energy levels of the InAs/GaAs quantum dots are calculated by implementing the k.p method. The calculated results show the importance of strain and piezoelectric effects.

Keywords: Quantum dot, k.p method, strain distribution and piezoelectricity.

1. Introduction

In recent years, the low-dimensional semiconductor nanostructures such as quantum wells and quantum dots (QDs) have attracted much attention in both experimental and theoretical researches [1-4]. Various semiconductor devices built from quantum dots have been studied, e.g., light emitting diodes and laser diodes [5-8]. Quantum dots can be produced by means of the Stranski-Krastanov process which uses the relief of elastic energy when two materials with a large lattice mismatch form an epitaxial structure [9]. In order to understand the electronic properties of the quantum dots, there are several approaches. In this work, we have calculated the single-particle electron and hole states and wave functions by implementing the k.p method because of the advantage to handle the computations in large sizes of quantum dots.

The aim of this study is to theoretically investigate the effect of strain and piezoelectricity on the electronic structures of self-assembled InAs/GaAs quantum dots. We calculate the energy trends as a function of dot sizes with and without

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including the strain field and piezoelectricity. Finally, the wave functions of electron and hole states are evaluated with and without the piezoelectricity.

2. 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. Continuum elasticity (CE) is determined to study. The total strain energy in the CE model is given by [3, 9]:

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

For a given structure, U_{CE} is minimized by using finite differences for the strains. The strain and the stress can be expressed as

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

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 calculation.

Piezoelectricity

The strain in quantum dot causes the atoms in the structure to change the crystal lattice geometry [10-12]. These changes can guide to the polarization in this structure. The piezoelectricity is defined as the creation of electric polarization by the application of stress to a crystal lacking a center of symmetry.

The piezoelectric potential is obtained by solving Poisson's equation.

$$\nabla^2 V_{pz} = \frac{\rho}{\varepsilon(r)}$$

Where V_{pz} is the piezoelectric potential. ρ is the piezoelectric charge defined as :

$$\rho = -\nabla \cdot P$$

And P is the polarization given by:

$$P = 2e_{14}\begin{vmatrix} e_{yz} \\ e_{xz} \\ e_{xy} \end{vmatrix}$$

Where e_{yz}, e_{xz} and e_{xy} are the off-diagonal components of the strain tensors and e_{14} is the piezoelectric constant of the considered material. $\varepsilon(r)$ is the static dielectric constant of the respective material at the position r. The parameters used to calculate the piezoelectricity are expressed in Table I. The piezoelectric potentials can be obtained by solving the 3D Poisson's equation in the path of the finite difference method. The piezoelectric potential is incorporated to k.p Hamiltonian as a diagonal term [13]:

$$H = H_{k.p} + V_{pz}I$$

Where $H_{k.p}$ is the k.p Hamiltonian and I is the identity matrix.

Electronic structure

In order to study the electronic properties of quantum dots, the band structure of the materials is symmetrically understood. There are several theoretical calculations such as effective mass [14], tight-binding [15, 16], pseudopotential [17], k.p method [3] and density functional theory [18]. Each technique has their own path to theoretically calculate the band properties of semiconductors. However, they start from the fundamental equation, Schrodinger equation. In this work, we have implemented the two-band model and four-band model to investigate the electron and valence states of quantum dots, respectively.

In two-band model, the wave functions of the electron states are a linear combination of the conduction bands given by:

$$\psi^e_{i_e}(\vec{r}) = \sum_{s_z=\pm 1/2} g^e_{i_e,s_z}(\vec{r})u_{s;s_z}(\vec{r})$$

Where $s = 1/2, s_z = \pm 1/2$

$$|u_{1/2;+1/2}> = s\uparrow$$

$$|u_{1/2;-1/2}> = s\downarrow$$

$g^e_{i_e,s_z}$ is the coefficient

In four-band model, the wave functions of the valence states are a linear combination of the valence bands defined as:

$$\psi_{i_v}^{v}(\bar{r}) = \sum_{j_z=\pm 1/2,\pm 3/2} g_{i_v,j_z}^{v}(\bar{r})u_{j;j_z}(\bar{r})$$

Where

$$\text{Heavy hole}\,|3/2;+3/2> = \frac{i}{\sqrt{2}}[|X\uparrow> + i|Y\uparrow>]$$

$$\text{Light hole}\,|3/2;+1/2> = \frac{i}{\sqrt{6}}[|X\downarrow> + i|Y\downarrow> - 2|Z\uparrow>]$$

$$\text{Light hole}\,|3/2;-1/2> = \frac{i}{\sqrt{6}}[|X\uparrow> - i|Y\uparrow> + 2|Z\downarrow>]$$

$$\text{Heavy hole}\,|3/2;-3/2> = -\frac{i}{\sqrt{2}}[|X\downarrow> + i|Y\downarrow>]$$

g_{i_v,j_z}^{v} is the coefficient

3. Results and Discussion

Strain distribution and Piezoelectricity

We have analyzed the strain distribution and the piezoelectricity in pyramidal InAs/GaAs quantum dot. To model the structure, we choose a finite GaAs zinc-blende lattice within a box with the boundary conditions. Within this box, we consider an InAs base width of 10.0 nm and height of 3.0 nm.

To consider strain influence on InAs/GaAs quantum dot, the knowledge of the strain tensors is essential. We have calculated the strain tensors at the middle of the y axis scanning along x and z directions. The contour plots of the strain tensors e_{xx}, e_{yy} and e_{zz} are visualized in Figure 1, 2 and 3, respectively. Below the InAs quantum dot, e_{xx} and e_{yy} are positive, while e_{zz} is negative. In the base region of the quantum dot, the situation is reversed. e_{xx} and e_{yy} are negative in the dot area and becomes positive at the top of quantum dot because GaAs substrate compresses the InAs dot mainly along the z direction. e_{zz} in Figure 3 is positive at the base of quantum dot. With increasing height within the dot, e_{zz} changes its sign and becomes negative at the top of the dot. At the top of dot, the force acting on the dot originates from the GaAs surrounding material. It causes the e_{zz} become negative and e_{xx} and e_{yy} become positive.

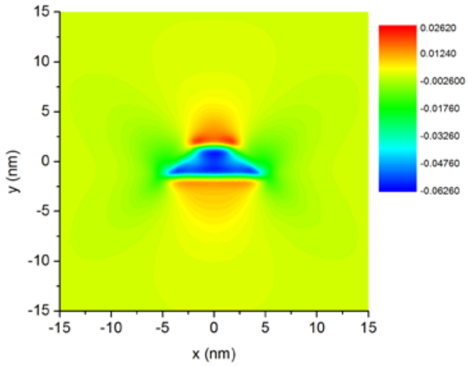

Figure 1. 2D plot of e_{xx}.

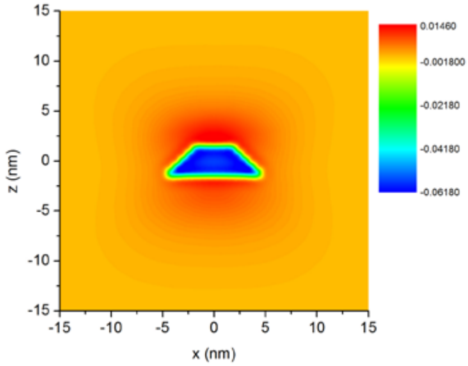

Figure 2. 2D plot of e_{yy}.

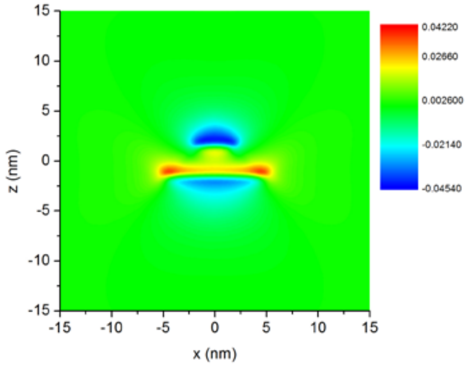

Figure 3. 2D plot of e_{zz}.

Then we have calculated the piezoelectric potential in InAs/GaAs quantum dot by solving the corresponding 3D Poisson's equation. We plot the isosurface of the piezoelectric potential. It shows that the piezoelectric potential is concentrated in the region close to the top and bottom of the pyramid. It illustrates that the piezoelectric potential is mostly positive (red isosurface) along the $[1\bar{1}0]$ direction and negative (blue isosurface) along the [110] direction. The isosurface potentials are ± 30 meV. This calculation introduces C_{2v} symmetry [3, 4].

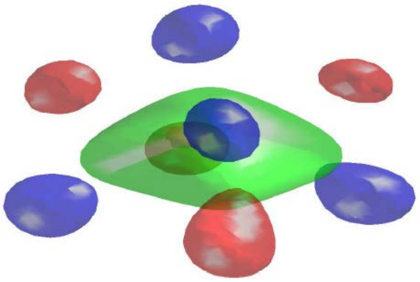

Figure 4. 3D plot of the piezoelectric potential of InAs/GaAs quantum dot.

Electronic structure

The electronic structure of InAs quantum dot in GaAs surrounding material has been studied by means of k.p calculation. The shape of quantum dot in this calculation is truncated pyramid. The base width is b nm and the height of the dot is 3.0 nm. The energy spectra of electron and hole states are plot as a function of the dot base widths in Figure 5 and 6, respectively. To investigate the influence of the strain field, these calculations are done in the presence and in the absence of strain effects. The numerical results demonstrate that the strain distribution in the quantum dot and surrounding material has a dominant influence on the electronic structure. The energies of electron and hole states taking into account the strain effect are shifted into the high energy side in comparison with ones without considering the strain effect. The graphs also show that the electron energies decrease with increasing the base widths, while the hole energies become rising as a function of the increasing base widths. Therefore, the band gap energies are reduced. The size-dependent property can be used to tune the band gap energies of the quantum dots.

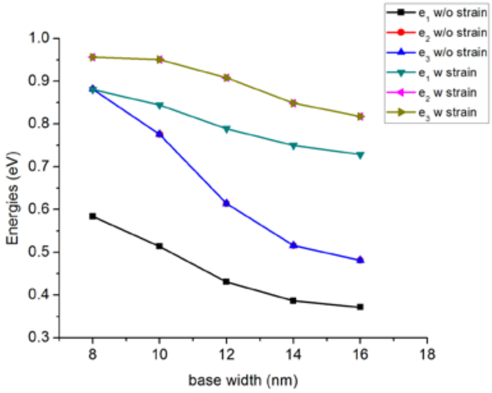

Figure 5. Electron energies of InAs/GaAs quantum dot as a function of dot sizes.

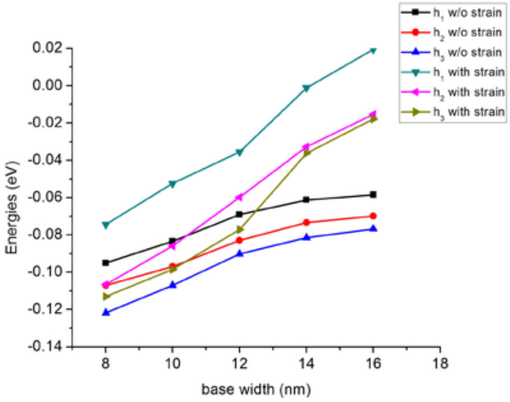

Figure 6. Hole energies of InAs/GaAs quantum dot as a function of dot sizes.

Finally the piezoelectricity (Pz) is examined. We consider the truncated pyramidal QD, basex = basey = 10.0 nm and height = 3.0 nm. The piezoelectric potential is included into the Hamiltonian. With the piezoelectricity, the electron and hole energies shift down about 10 meV which are very small compared to the strain field. The wave functions of electron and hole states are revealed as 2D plot along the x and y axis in Figure 7 and 8, respectively. The wave functions of QD are evaluated with and without the piezoelectric potential. The piezoelectric potential does not change the orientation of the s-electron states (e_1) as shown in Figure 7. In the p-electron states (e_2 and e_3), the piezoelectricity has flipped the orientations of wave functions from

$[1\bar{1}0]$ to [110] and vice versa. The changes of the orientations also happen in the valence states of quantum dots because hole sates consist of of the linear combination of the p orbitals. The inclusion of the piezoelectricity into quantum dot introduces C_{2v} symmetry.

Table 1. Material parameters for the calculation.

	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

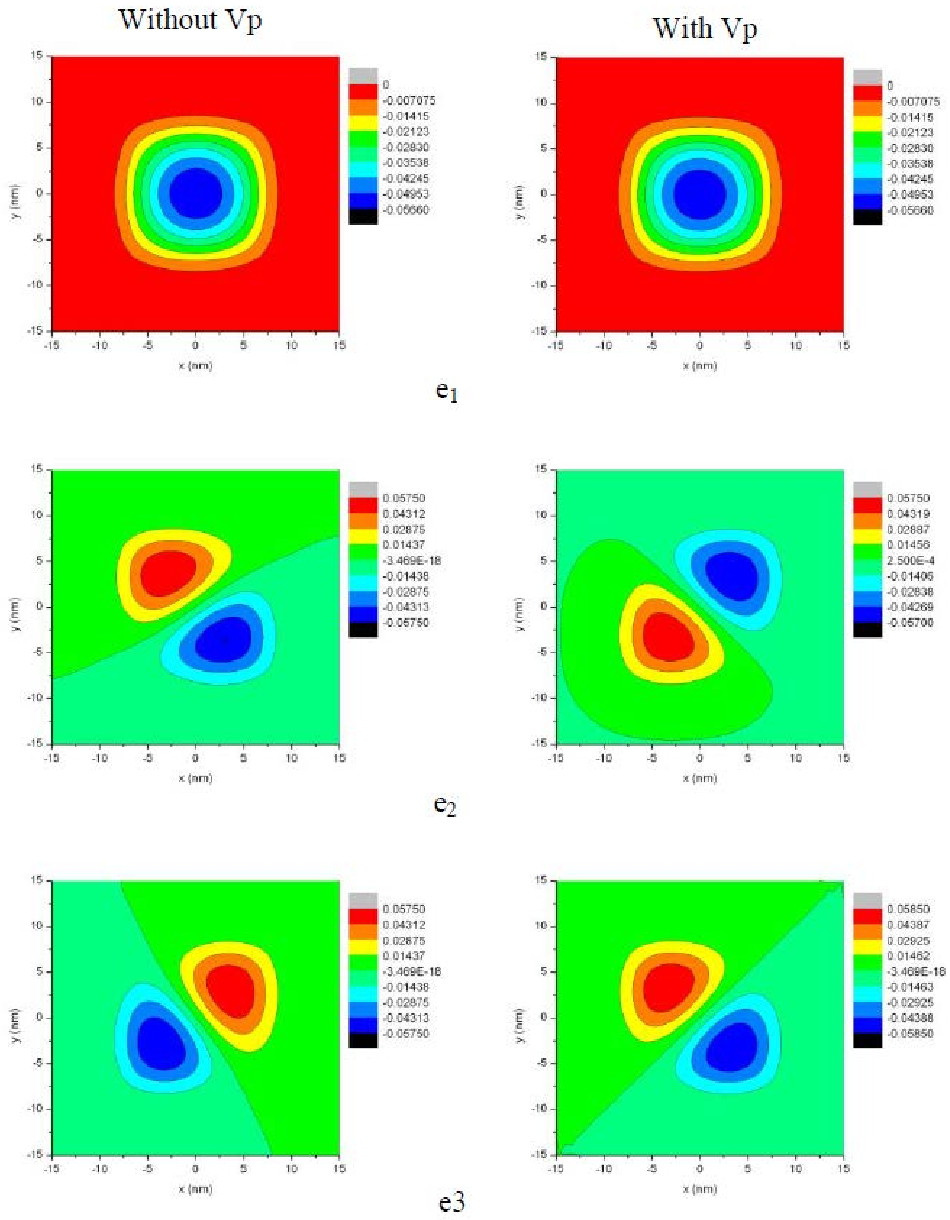

Figure 7. 2D plot of electron wave functions w/o and with the Piezoelectricity (Pz).

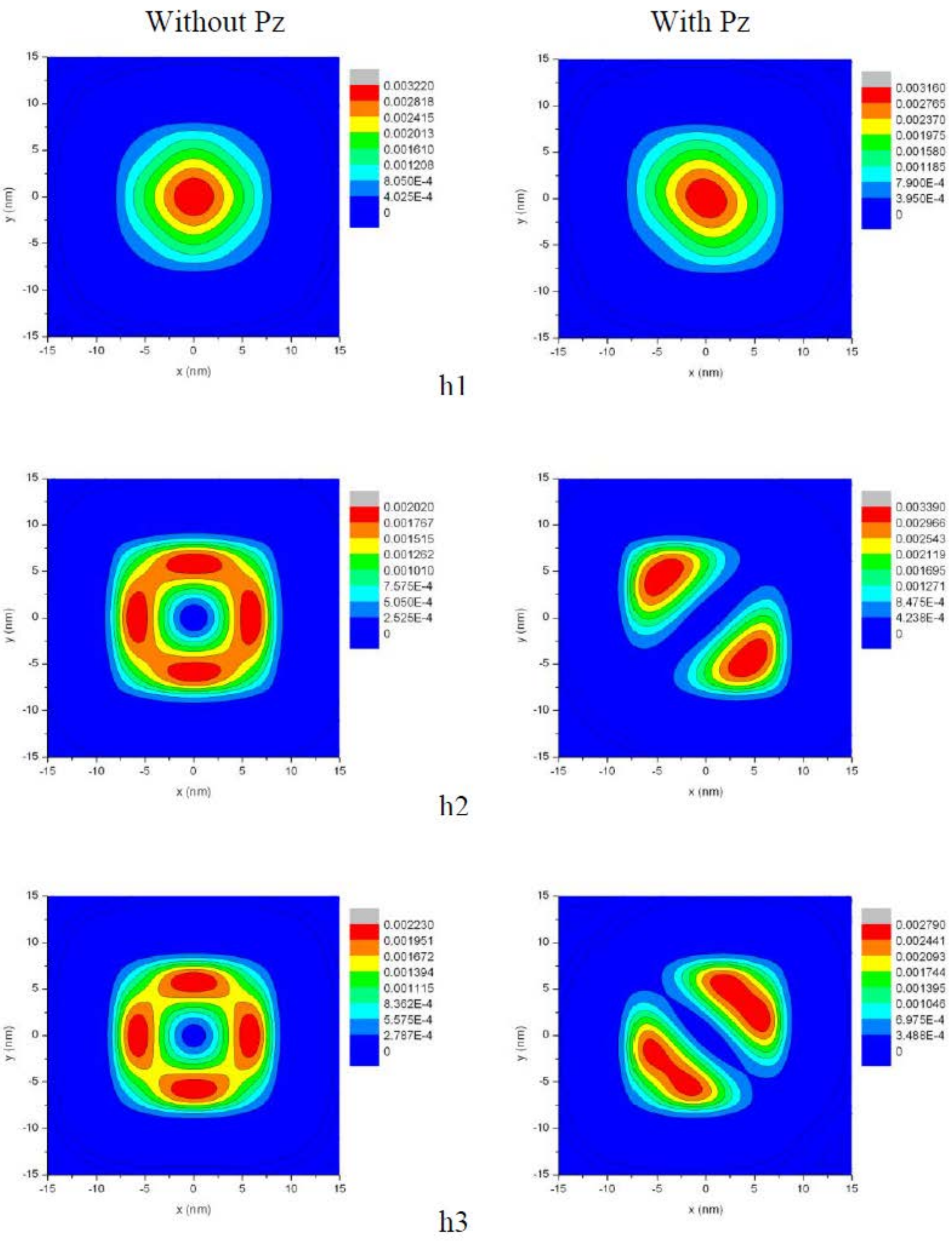

Figure 8. 2D plot of hole wave functions w/o and with the Piezoelectricity (Pz).

5. Conclusions

The effect of the strain and piezoelectricity of self-assembled InAs/GaAs quantum dots has been theoretically investigated by means of the continuum elastic theory and k.p method. The calculated results show the importance of strain and piezoelectric effects on the electronic structure. The energies of electron and hole states including the strain effect are shifted into the high energy side in comparison with ones excluding the strain effect. The piezoelectric potential does not change the orientation of the s-electron states (e_1), while the p-electron states (e_2 and e_3) flip the orientations of wave functions from $[1\overline{1}0]$ to [110] and vice versa.

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