Piezoelectric effects and electronic structures of InAs/GaAs quantum dots grown along (111) and (011) directions*

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Piezoelectric effects and electronic structures of InAs/GaAs quantum dots grown along (111) and (011) directions are investigated in this paper. The finite element method is used. Electronic energy levels are calculated by solving the three-dimensional effective mass Schrödinger equation including a strain modified confinement potential and piezoelectric effects. The difference in electronic structure between quantum dots grown along the (111) direction and the (011) direction are compared. The cubic and truncated pyramidal shaped quantum dots are adopted.

Keywords: quantum dot, electronic structure, piezoelectric effect

PACC: 7320D, 0365, 4620

1. Introduction

Quantum dots (QDs) have attracted great attention due to the possibility of fabricating coherent and dislocation-free semiconductor devices, and also to the possible applications in optoelectronic and microelectronic fields.[1−4] Among the materials, self-assembled InAs/GaAs QDs have received considerable attention because of their successful applications in photovoltaic and photonic devices.

Nowadays it is a core issue to optimize the properties of QDs. Many studies focused on the electronic structures of InAs/GaAs QDs grown along the (001) direction,[5,6] but little effort was made to study the electronic structures of QDs grown along the (111) or (011) direction.[7] Theoretical and experimental studies show that optical properties of QDs are strongly dependent on the geometric parameters of QDs. Recent experiments demonstrated that the growth direction could affect the shapes and crystal qualities of QDs.[8] The choice of an appropriate growth direction is conducive to improving uniformities and crystal qualities of QDs, enhancing the light-emitting intensity, and preventing the photoluminescence spectra from broadening. The InAs/GaAs QDs grown along the (111) and the (011) directions can possess excellent characteristics for semiconductor quantum devices, therefore it is necessary to study the electronic structures of InAs/GaAs QDs grown along these directions.

In this paper, we calculate electronic structures of InAs/GaAs QDs grown along the (111) and the (011) directions, with the consideration of the band edge modification induced by the strain and piezoelectric effects. We use the continuum elastic theory to determine the strain distributions. The piezoelectric effect is considered by introducing a piezoelectric potential into the Schrödinger equation. Our results show that the piezoelectric effects and electronic structures of QDs are closely related to the growth direction.

2. Numerical calculations

2.1. Strain distribution

The dependence of stress components on strain components can be set up by using a stiffness matrix D, and the strain and the stress can be expressed as[9−12]

$$\varepsilon_{ij} = \left(\frac{\mathrm{d}u_i}{\mathrm{d}x_j} + \frac{\mathrm{d}u_j}{\mathrm{d}x_i} \right) /2 \,, \tag{1a}$$

and

$$\sigma = D(\varepsilon - \varepsilon_0) + \sigma_0 \,. \tag{1b}$$

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For the InAs/GaAs material along (001), (010) or (100) directions the D matrix can be expressed as

$$D = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}. \quad (2)$$

As for materials grown along other directions, we need a tensor transformation[13] to obtain the right stiffness matrix D

$$C_{i,j,k,l} = U_{i,m}U_{j,n}U_{k,o}U_{l,p}C_{m,n,o,p}, \quad (3)$$

where i, j, k, l are in x', y', z' coordinate system, and m, n, o, p are in x, y, z coordinate system. The $U_{i,j}$ is one of the components of the rotation matrix which is related to different coordinates, and it is given as follows:

$$U = \begin{pmatrix} \cos\phi\cos\theta & \sin\phi\cos\theta & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \\ \cos\phi\sin\theta & \sin\phi\sin\theta & \cos\phi \end{pmatrix}. \quad (4)$$

The relations between the two coordinates and the angles can be seen in Fig. 1.

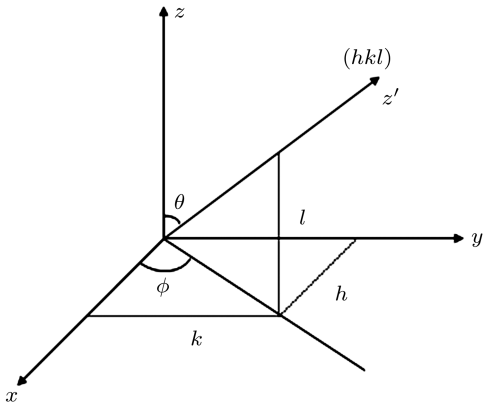


Fig. 1. Coordinate transformation, where (hkl) is along the growth direction.

The elastic constants of InAs and GaAs along the (111) and (011) directions are

$$C_{\mathrm{InAs}(111)} = \begin{pmatrix} 103.87 & 38.4 & 31.54 & 0 & 9.699 & 0 \\ 38.4 & 103.87 & 31.54 & 0 & -9.699 & 0 \\ 31.54 & 31.54 & 110.72 & 0 & 0 & -9.699 \\ 0 & 0 & 0 & 25.3 & 0 & 0 \\ 9.699 & -9.699 & 0 & 0 & 25.3 & 0 \\ 0 & 0 & 0 & -9.699 & 0 & 32.95 \end{pmatrix} (10^9\ \mathrm{N/m^2}), \quad (5)$$

$$C_{\mathrm{GaAs}(111)} = \begin{pmatrix} 145.7 & 44.8 & 35.8 & 0 & 12.7 & 0 \\ 44.8 & 145.7 & 35.8 & 0 & -12.7 & 0 \\ 35.8 & 35.8 & 154.6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 41.5 & 0 & -12.7 \\ 12.7 & -12.7 & 0 & 0 & 41.5 & 0 \\ 0 & 0 & 0 & -12.7 & 0 & 50.4 \end{pmatrix} (10^9\ \mathrm{N/m^2}), \quad (6)$$

$$C_{\mathrm{InAs}(011)} = \begin{pmatrix} 103.9 & 45.3 & 24.7 & 0 & 0 & 0 \\ 45.3 & 83.3 & 45.3 & 0 & 0 & 0 \\ 24.7 & 45.3 & 103.9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 39.6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 19.0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 39.6 \end{pmatrix} (10^9\ \mathrm{N/m^2}), \quad (7)$$

$$C_{\mathrm{GaAs(011)}} = \begin{pmatrix} 145.7 & 53.8 & 26.9 & 0 & 0 & 0 \\ 53.8 & 118.8 & 53.8 & 0 & 0 & 0 \\ 26.9 & 53.8 & 145.7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 59.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 32.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 59.4 \end{pmatrix} (10^9\ \mathrm{N/m^2}). \tag{8}$$

The elastic energy of the system can be written as

$$E_{\mathrm{e}} = \frac{1}{2}\int \sigma^{\mathrm{t}}(\varepsilon - \varepsilon_0)\mathrm{d}V\ , \tag{9}$$

where ε_0 is the initial strain in the QD system. It is the lattice mismatch of the material in the QD region, and its value is zero in the surrounding barriers.

2.2. Electronic structure

Piezoelectricity is defined as the electric polarization generated after applying a stress to a crystal that lacks a symmetric centre.[14−16] For the InAs/GaAs system, the strain induced polarization P can be expressed as

$$P = (2e_{14}) \begin{pmatrix} \varepsilon_{yz} \\ \varepsilon_{xz} \\ \varepsilon_{xy} \end{pmatrix}. \tag{10}$$

Piezoelectric charge density resulting from the polarization can be written as

$$\rho = -\boldsymbol{\nabla} \cdot \boldsymbol{P}. \tag{11}$$

In the absence of external charges, the resulting piezoelectric potential V_{p} can be obtained by solving Poisson's equation,

$$\varepsilon_0 \nabla \cdot (\varepsilon_r(r)\nabla V_{\mathrm{P}}) = \rho\ , \tag{12}$$

where ε_0 and ε_r are the dielectric constant in vacuum and the relative static dielectric tensor respectively.

We consider the one-band effective mass envelope function formalism with the modified band edge from the eight-band $k \cdot p$ theory. The electron Hamiltonian can be written as

$$H_{\mathrm{e}} = -\frac{\hbar^2}{2m_{\mathrm{e}}^*}\nabla^2 + E_{\mathrm{c}}^* - eV_{\mathrm{p}}, \tag{13}$$

where E_{c}^* is the strain modified conduction-band edge. The values used in this paper are given in Table 1.

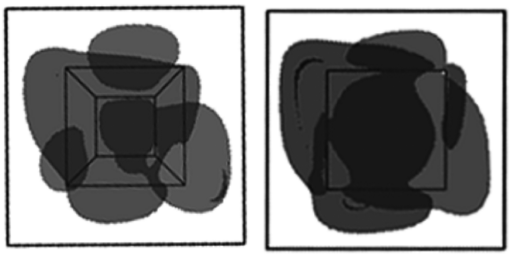
Once the strain distribution is calculated by using the finite element method, the piezoelectric potential can be obtained from Eqs. (12) and (13) directly by solving the Poisson's equation. Then the electronic energy levels can be calculated by using the piezoelectric potential V_{p}.

Table 1. Material parameters[5,17] used for calculation.

	C_{11}/GPa	C_{12}/GPa	C_{44}/GPa	ε_{r}	$e_{14}/\mathrm{C\cdot m^{-2}}$	m_{e}^*/m_0	E_{c}^*/eV
InAs	83.3	45.3	39.6	14.6	-0.115	0.022	0
GaAs	118.8	53.8	59.4	13.18	-0.230	0.067	0.395

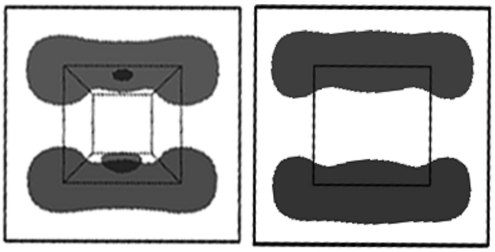
3. Results and discussion

Figures 2(a) and 2(b) depict the polarization distributions of truncated pyramidal and cubic QDs grown along the (111) direction, respectively. It is shown that the piezoelectric potential is mainly distributed around the QD and the wetting layer. As can be seen, the polarization distribution is dependent on the shape of the QD. Figure 3 shows the polarization distribution along the (011) direction. Comparing Fig. 3 with Fig. 2, we can obtain the conclusion that the polarization distribution strongly depends on growth direction. The piezoelectric potential of a truncated pyramidal shaped QD is 0.0441 eV and –0.0796 eV along the (111) direction and 0.0541 eV and –0.0552 eV along the (011) direction. Comparing the results with those given in Ref. [9] clearly shows that the piezoelectric effect in InAs/GaAs QD is weaker than that in GaN/AlN QD.



(a) (b)

Fig. 2. Polarization distributions of (a) pyramidal dot and (b) cubic dot grown along (111) direction.



(a) (b)

Fig. 3. Polarization distributions of (a) pyramidal dot and (b) cubic dot grown along (011) direction.

The strain modified conduction band edges are shown in Fig. 4. It can be seen that the polarization effect increases the barrier of a QD. A comparison between Fig. 4(a) and Fig. 4(b) shows that the piezoelectric effect can more strongly influence the properties of a QD grown along the (111) direction than that grown along the (011) direction. Figure 5 shows the electron density distributions of truncated pyramidal shaped QDs for the ground state in the conduction band along the (111) and the (011) directions. The electron wavefunction of a QD grown along the (111) direction has an upward displacement compared with that grown along the (011) direction. The reason is that piezoelectric effects more strongly influence the properties of a QD grown along the (111) direction than that grown along the (011) direction. The ground state and the lowest two excited state energy levels are 0.219432, 0.379141 and 0.383134 eV along the (111) direction, and 0.205527, 0.354941, 0.365058 eV along the (011) direction. It can be seen that QDs grown along the (111) direction have higher energy levels than those grown along the (011) direction. We have also calculated the cubic QDs and obtained the same conclusion.

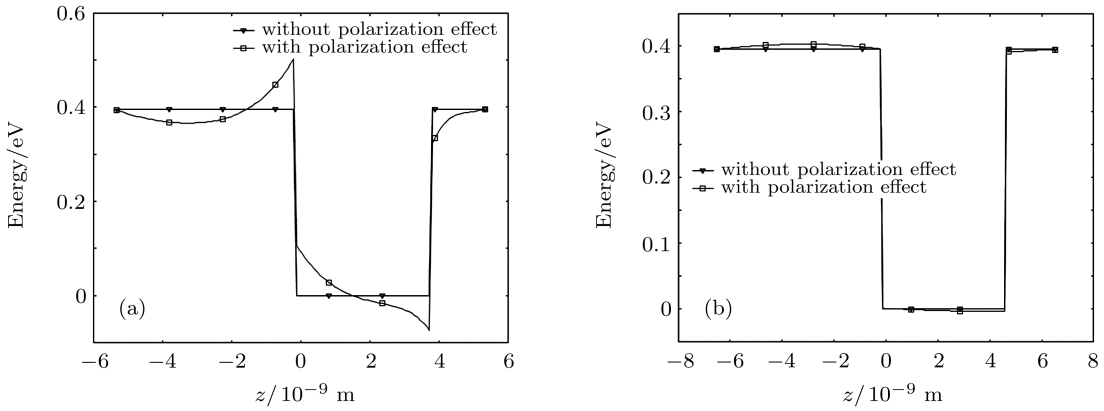
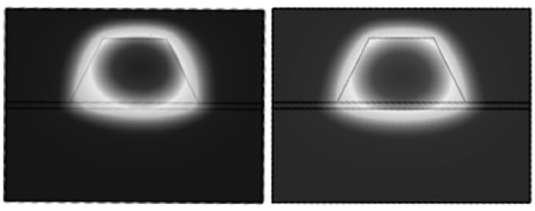


Fig. 4. Polarization modified conduction-band (CB) energies of truncated pyramidal shaped QDs along (a) (111) and (b) (011) directions.



(a) (b)

Fig. 5. Electron probability density distributions of truncated pyramidal shaped QDs for the ground state (a) along (111) direction, (b) along (011) direction.

4. Conclusion

The piezoelectric effects and the electronic structures of InAs/GaAs QDs grown along (111) and (011) directions are calculated. Both the cubic and the truncated pyramidal shaped QDs are discussed. By taking into account the influence of strain and the piezoelectric potential, we solve a three-dimensional, effective-mass single-band Schrödinger equation for electronic energy levels. The results show that piezoelectric ef-

fects and the electronic structures of QDs are closely related to the growth direction. Quantum dots, rather than spherical shaped, grown along the (111) direction have higher energy levels than those grown along the (011) direction, with their volumes being the same. The conclusion is useful for further analysing the semiconductor quantum devices and photonic devices. For future research it is interesting to analyse the spectrum characteristics and the optical transition rates of QDs grown along these directions.

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