Influence of nanomechanical force on the electronic structure of InAs/GaAs quantum dots*

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We show nanomechanical force is useful to dynamically control the optical response of self-assembled quantum dots, giving a method to shift electron and heavy hole levels, interval of electron and heavy hole energy levels, and the emission wavelength of quantum dots (QDs). The strain, the electron energy levels, and heavy hole energy levels of InAs/GaAs(001) quantum dots with vertical nanomechanical force are investigated. Both the lattice mismatch and nanomechanical force are considered at the same time. The results show that the hydrostatic and the biaxial strains inside the QDs subjected to nanomechanical force vary with nanomechanical force. That gives the control for tailoring band gaps and optical response. Moreover, due to strain-modified energy, the band edge is also influenced by nanomechanical force. The nanomechanical force is shown to influence the band edge. As is well known, the band offset affects the electronic structure, which shows that the nanomechanical force is proven to be useful to tailor the emission wavelength of QDs. Our research helps to better understand how the nanomechanical force can be used to dynamically control the optics of quantum dots.

Keywords: nanomechanical force, quantum dots, energy levels, electronic structure

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1. Introduction

Recently, self-assembled semiconductor quantum dots (QDs) have attracted intense attention because of their potential applications in photonics, sensors, quantum information, and precision measurements.[1–3] The electronic structure of a semiconductor QD is a direct factor influencing QD optical properties. There are mainly two kinds of methods: passive control and active control. The passive control is obtained by tailoring dot size, shape, and composition via growth. The ways of active control include improving nanomechanics, electric field,[4–7] and magnetic field.[8] An imposed nanomechanical strain[9–12] provides a route to dynamically re-engineering QD structural symmetry in order to control excitations, polarize transitions, tune exchange splitting, induce entanglement, or modify coupling between QDs. Those capabilities are needed to use QDs in nanophotonics, quantum information processing and in optically active devices, such as optomechanical cavities[13,14] and semiconductor nanotubes.[15–18]

The nanomechanical force is being studied for mass sensing,[19,20] mechanical computing,[21,22] and energy harvesting.[23] To approach the quantum limit of metrology and to provide coherent transducers that couple classical machines to quantum devices, structures are cooled.[24–27] To exploit hybrid nanomechanical-QD devices, fundamental understandings are needed. The connections between the strains of lattice mismatch and imposed nanomechanical strain and carrier states of QDs in nanomechanical devices in excited QDs need to be understood. We study pyramidal InAs/GaAs QD subjected to the nanomechanical force in the vertical direction along the z axis. The QD system is bent upward or downward depending on vertical directions. Strain distributions, electrons and holes are redistributed vertically along the QD growth axis or horizontally in the plane of the QD, depending on how the nanomechanical force is applied.

In this paper, the nanomechanical force affecting the electric structure of a semiconductor QD is mainly discussed. When there is nanomechanical force on QD system, both the nanomechanical force and the lattice mismatch influence the QD system, which results in the lattice inside the QD system presenting larger deformation when the atoms reach balance. At this moment, accumulation strain inside the QD system affects the carrier band greater than lattice mismatch. For a small InAs/GaAs QD, piezoelectric effects are ignored because they are small. When the nanomechanical force is greater than a certain value, the atoms inside the QD system would increase in deformation, which leads to defect. The values of mechanics are lower than the critical limit, and the defect inside the QD system is not considered in the paper.

The finite element method (FEM) of calculating the strain distribution, the continuous elastic theory, and the single band $k \cdot p$ theory are used, and the pyramidal structure model is

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adopted in Section 2. In Section 3, we present the strain profiles, the confined energy levels of both electrons and heavy holes of QDs and the intervals of electron and heavy hole energy levels. First we discuss the strain distribution in mechanically strained QDs. Next, we show carrier energy level shift and the interval of electron energy levels and heavy hole energy levels under nanomechanical strain variation. We also explain the reason why these levels shift with the nanomechanical force in the local band profile. Finally, the conclusion is drawn.

2. Geometric structure models and theoretical methods

The pyramid QD structure model with mechanics is shown in Fig. 1. The materials of substrate and capping layer are GaAs and materials of QD and wetting layer are InAs. Size parameters are as follows: for each of the substrate and capping layers, the length is 200 nm, the width is 40 nm, and the thickness is 10 nm; for QD, the length is 200 nm, the width is 40 nm, the bottom radius is 10 nm, and the top radius is 4 nm; for the wetting layer, the length, width, and thickness are 200 nm, 40 nm, and 1 nm separately. There are $F_{\rm up}$ forcing on the upper surface and $F_{\rm down}$ forcing on the lower surface. The surfaces along the x axis are both fixed and the other surfaces are free.

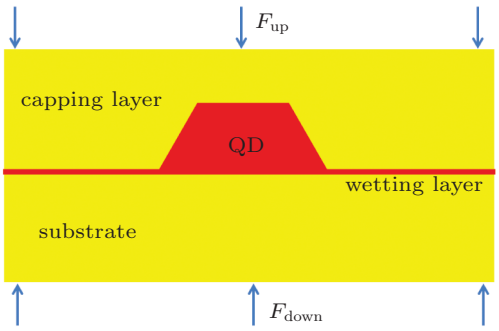


Fig. 1. (color online) Profile of QD with mechanics.

In this paper we use the FEM to investigate the strain distributions of self-organized QDs structures according to the continuum elasticity theory.[28,29] The FEM calculated strain distribution has been realized.[28] A comparison has been made between FEM and a more accurate atomic method, and the results show that only a little difference can be found near the boundary of the quantum dots.[28,29] The dependence of strain component on stress component can be set up by using a stiffness matrix $\boldsymbol{D}$. For InAs/GaAs as the cubic crystal, the $\boldsymbol{D}$ matrix can be expressed as

$$\boldsymbol{D} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}, \tag{1}$$

and then the stress and the strain may be expressed as two column vectors σ and ε:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{xz} \end{pmatrix} = \boldsymbol{D}(\varepsilon - \varepsilon_0) + \boldsymbol{\sigma}_0, \tag{2}$$

$$\varepsilon = \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{xy} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \end{pmatrix} = \begin{pmatrix} \partial u/\partial x \\ \partial v/\partial y \\ \partial w/\partial z \\ \partial u/\partial x + \partial u/\partial x)/2 \\ \partial v/\partial z + \partial w/\partial y)/2 \\ \partial u/\partial z + \partial w/\partial x)/2 \end{pmatrix}, \tag{3}$$

where u, v, and w are the displacements along the coordinates x, y, and z directions respectively, σ_0 is the initial stress and its value is zero, and the component of ε_0 is the initial strain in the quantum dot system. In a quantum dot region, the initial strain is the lattice mismatch of the hetero-structure material. At the surrounding barriers, the initial strain is zero. The lattice mismatch can be expressed as

$$\varepsilon_0 = \frac{\alpha_{\rm InAs} - \alpha_{\rm GaAs}}{\alpha_{\rm InAs}}. \tag{4}$$

The piezoelectric modified band is ignored in this paper because the piezoelectric effect on InAs/GaAs QD is not obvious. The boundary condition is that the bottom side is fixed while other sides are free, and the detailed operation steps are those as shown in Ref. [28].

Energies of the Brillouin zone center in a heterostructure semiconductor change because of strains. Without regard to shearing strain, based on the single-band $k \cdot p$ theory, the strain-modified energies are

$$E_{\rm c} = E_{\rm v,av} + \frac{\Delta}{3} + E_{\rm g} + \Delta E_{\rm c}, \tag{5}$$

$$E_{\rm hh} = E_{\rm v,av} + \frac{\Delta}{3} + \Delta E_{\rm hh}, \tag{6}$$

where $E_{\rm v,av}$ is the average valence band energy, Δ is the spin–orbit separation energy, $E_{\rm g}$ is the fundamental gap, $\Delta E_{\rm c}$ is the strain modified conduction band edge, and $\Delta E_{\rm hh}$ is the strain modified heavy hole band edge that can be expressed as

$$\Delta E_{\rm c} = a_{\rm c}\varepsilon_{\rm hyd}, \tag{7}$$

$$\Delta E_{\rm hh} = a_{\rm v}\varepsilon_{\rm hyd} - 0.5b\varepsilon_{\rm bi}, \tag{8}$$

with $a_{\rm c}$, $a_{\rm v}$, and b being the deformation potential constants, $\varepsilon_{\rm hyd} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$ being the hydrostatic strain and $\varepsilon_{\rm bi} = 2\varepsilon_{zz} - \varepsilon_{xx} - \varepsilon_{yy}$ meaning the biaxial strain.

The values used in this paper for all kinds of material parameters are given in Table 1.

Table 1. Material parameters. In the table, the abbreviation def. pot. is short for deformation potential.

	Quantity	Unit	GaAs	InAs
Lattice constant	α	nm	5.6503	6.0553
Fundamental gap	E_g	meV	1518.0	413.0
Averaged VB edge	E_V	meV	–6920	–6747
Spin–orbit coupling energy	Δ	meV	340	380
Optical matrix parameter	E_g	meV	28000	22204
CB effective mass	m_e	m_0	0.067	0.022
CB hydrostatic def. pot.	a_c	meV	–8013	–5080
VB hydrostatic def. pot.	a_v	meV	–1160	–1000
VB shear def. pot	b	meV	–2000	–1800
Elastic compliance	C_{11}	GPa	118.8	83.8
Elastic compliance	C_{12}	GPa	53.8	45.3
Elastic compliance	C_{44}	GPa	59.4	39.6

3. Results and discussion

The effects of both F_{up} and F_{down} on strain distribution, conduction band edge, and valance band edge are discussed. The detailed results are as follows.

As shown in Fig. 2, when $F = 0$ GPa, because of the mismatch strain, there is relaxation in the QD system (composed of substrate, capping layer, and QD) and then there is a tiny deformation in the bottom of the substrate. With F_{down} increasing, there are more deformations in the QD system. When the deformation is beyond the limit, there are lots of defects in the system, which results in the sample being damaged. When $F_{up} = 0.3$ GPa, the deformation in the system is large enough, so mechanical force selected is in a range of 0 GPa–0.3 GPa and it is assumed that mechanical force would not destroy the sample.

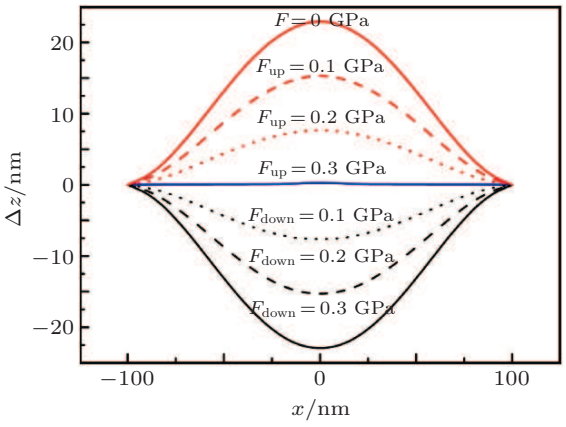


Fig. 2. (color online) Displacements of QD system subjected to the nanomechanical force along the z axis direction.

Firstly, strain distributions in a mechanically strained QD are discussed. The distributions of the biaxial strain and the hydrostatic strain are as shown in Fig. 3. When no mechanical force exists, lattice mismatch and mechanics both affect the strain inside the QD system, so the strain including lattice mismatch, which is inherent in InAs/GaAs QDs, the applied mechanical strain and the resulting relaxation of the strains should be considered. When there is mechanical force on the QD system along the growing direction, the hydrostatic strain and the biaxial strain inside the QD are enhanced noticeably. For hydrostatic strain, it is clear to find that there are more obvious changes with F_{up} than those with F_{down} in the substrate closer to the QD, and the bigger the nanomechanical force, the larger the variation is. The hydrostatic strain is influenced by F_{down} more obviously in the capping layer. For biaxial strain, the strain increases with F_{up} increasing and decreases with F_{down} increasing in the substrate region, but in the capping layer region, the strain decreases with F_{down} increasing and augments with F_{up} increasing. When the QD system is pushed down, the upper half inside the QD is forced directly due to the pyramid structure, so the lattice along the vertical direction is due to the nanomechanical force and then the biaxial strain and the hydrostatic strain must increase correspondingly. When the lattice of the QD along the vertical direction is squeezed, the lattice inside the QD along the horizontal direction will present relaxation that is bigger than the compressive degree, so the hydrostatic and biaxial strains in the bottom half of QDs decrease correspondingly.

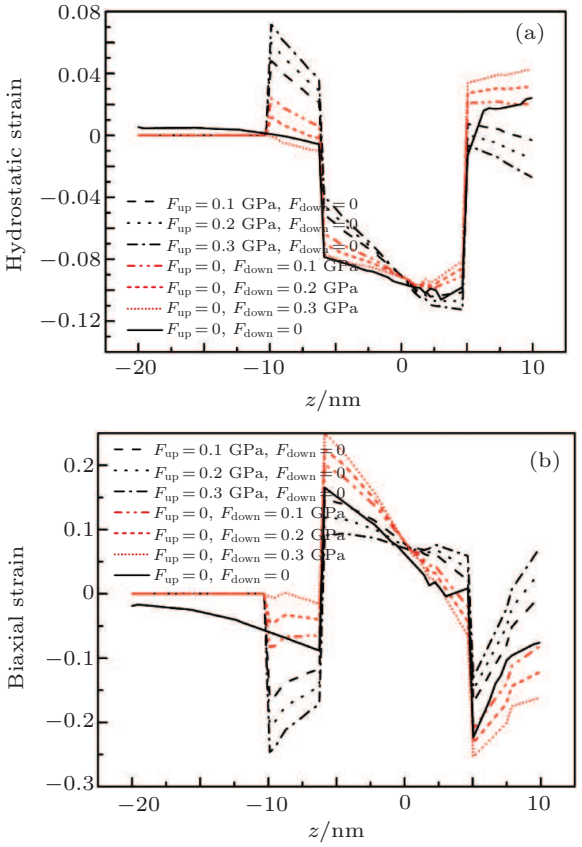


Fig. 3. (color online) Strain distributions of QD subjected to the nanomechanical force along the direction parallel to the z axis through the center of the pyramid: (a) the hydrostatic strain distributions with and without nanomechanical force, (b) the biaxial strain distribution with and without nanomechanical force.

Similarly, the strains in the substrate and capping layer regions are enhanced greatly when the QD system is bent up-

ward. In the QD region closer to the substrate, the QD system bending up enhances the relaxation degree along the horizontal direction of QD lattice, which leads to ε_{xx} and ε_{yy} decreasing and then the biaxial strain and the hydrostatic strain would decrease with mechanical force increasing. However, in the QD region closer to the capping layer, due to the substrate bending up, the top of the lattice is compressed greatly and the horizontal strain decreases. Since the decreasing degree of horizontal strain is larger than the increasing degree of vertical strain, the hydrostatic strain drops while the biaxial strain improves. The variations of the hydrostatic strain and the biaxial strain by mechanical force affect the confined potential of the electron and heavy hole indirectly.

Then, how the nanomechanical force influences the confined potential is studied. As illustrated in Fig. 4, in the substrate region, the band edge moves down while the band edge moves up in the capping layer region. However, in the top half part of the QD (close to the QD top) the band edge moves down but it moves up in the bottom half part of the QD (close to the QD bottom). There is tiny influence on valance band edge with nanomechanical force on the QD system. The valance band edge moves down in the substrate and moves up in the capping layer. The result of nanomechanical influence on the conduction band edge is the same as on the valance band edge inside QD. In Fig. 4, the band edge shifts more obviously with larger nanomechanical force, so the nanomechanical force selected in this paper needs to be in a suitable scope due to the deformation limit of the QDs system.

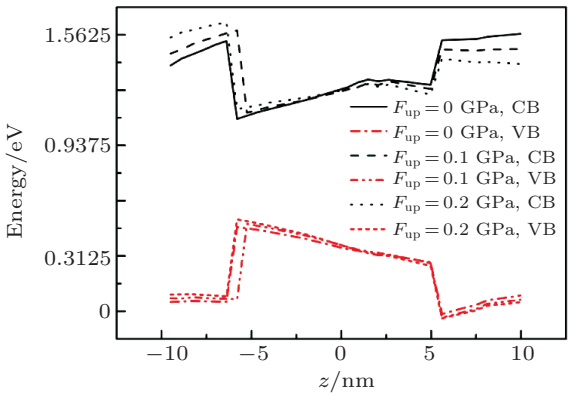


Fig. 4. (color online) Conduction band edge and valance band edge profiles of QD along the direction parallel to the z axis through the center of the pyramid with and without nanomechanical force.

It is shown in Fig. 5 how nanomechanical force influences electron and heavy hole energy levels. As illustrated in Fig. 5, both F_{up} and F_{down} result in improving the electron ground state level. The energy levels are more sensitive when QD is bent upward because F_{up} affects the strain more obviously as shown in Fig. 3. For the first excitation state, the varying rule of electronic energy increases and then decreases with mechanical force increasing. When mechanical force is greater than 0.21 GPa, the first excitation state level decreases. The interval between the ground state level and the first excitation state level becomes smaller, which explains that the influence of QD luminescence characteristic affected by mechanical force is nonlinear in terms of transition luminescence inside the electronic belt.

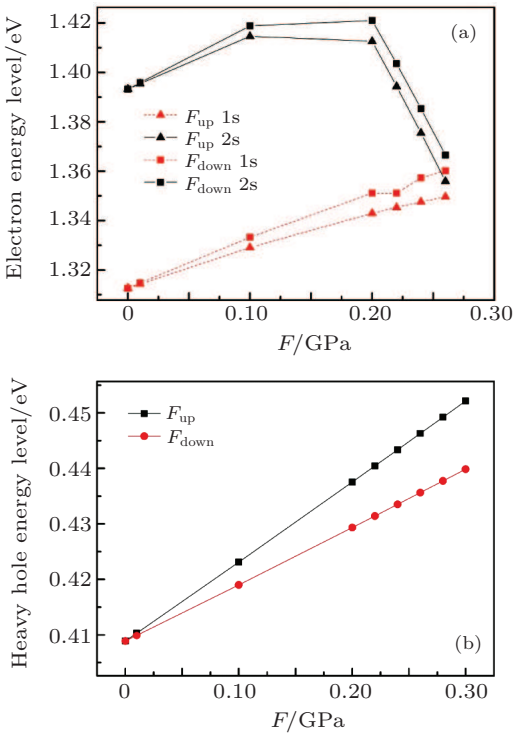


Fig. 5. (color online) Relations between the carrier energy levels and mechanics: (a) the relation between electron energy levels and nanomechanical force, and (b) the relation between the ground state of heavy hole energy levels and nanomechanical force.

The interval between the ground state level and the first excitation level improves and then drops with nanomechanical force increasing, and the interval reaches maximum when mechanical force is in a range of 0.1 GPa–0.2 GPa. There are still more effects on the first excitation state level by F_{up} than by F_{down}.

In Fig. 5, the ground state energy of QD heavy hole is enhanced linearly with mechanical force increasing. It is easy to find that the variation of QD heavy hole energy by F_{down} is more obvious than by F_{up}. The ground state energies of electron and heavy hole influence QD luminescence characteristic mainly and the interval between them represents the luminescence wavelength of QD approximately, so the luminescence wavelength of QD would present a blueshift with mechanical force increasing.

The results of nanomechanical force affecting the interval between the ground state energies of electrons and heavy holes are shown in Fig. 6. The value of energy interval increases with F_{up} increasing while the value of energy increases and then decreases with F_{down} improving. In the case of F_{down} equal to F_{up}, the influence of F_{down} on energy is greater. In

terms of band-to-band transition, the steering capacity of QDs luminescence wavelength by F_{down} is stronger than that by F_{up}.

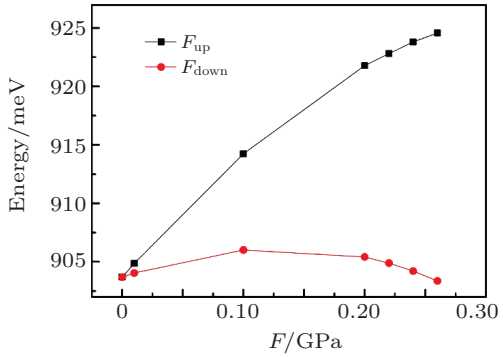


Fig. 6. (color online) Varying disciplines of the interval between ground state energies of electrons and heavy holes considering nanomechanical force.

4. Conclusion

In this work, we obtain some interesting and meaningful conclusions as summarized below by investigating the strain and electronic structure of InAs/GaAs (001) QD subjected to nanomechanical force in the vertical direction along the z axis. We show how the nanomechanical force can be used to dynamically control the optics of quantum dots. Hydrostatic and biaxial strain distributions can shift together in the same direction or in opposite directions, depending on how mechanical force is applied, which results in variations of electron and heavy hole energy levels distributions. The internal strain due to the lattice mismatch, the nanomechanical strain, and the applied strain that can be minimized by the internal readjustment are all accounted for to model correctly the strain effects. Furthermore, the interval of electron and heavy hole levels changes with mechanical force, which leads to the shifting of the emission wavelength of QDs. The result of the carrier energy level varying with nanomechanical force provides a control method to tune QD optical properties.

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