Influence of the strain on the energy levels of semiconductor quantum dots

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We systematically investigate a strain of self-assembled InAs/GaAs quantum dots (QDs) for the case of growth on a (001) substrate. The dependence of the biaxial and hydrostatic components of the strain on the quantum dot aspect ratio is studied using a finite element method. The dependence of the carrier's confining potentials is then calculated in the framework of eight-band $\vec{k}\cdot\vec{p}$ theory. The shifts of the energy level in three shapes of QDs are investigated. By comparing the results, the influence of the strain on the QDs are given.

OCIS codes: 160.6000, 130.5990, 140.5960, 160.3380.

Nanometer-size semiconductor quantum dots (QDs) are the subject of a rapidly developing area in semiconductor research, as they provide an increase in the speed of operation and a decrease in the size of semiconductor devices. As we know, semiconductor QD is grown by S-K mode, because of the lattice mismatch between deposited material and substrate, the system is under high strain. The strain is therefore a key feature of the dots and causes large change in band profiles. It is important to analyze this problem for QD device using, and this problem has been discussed widely[1−3]. The research is concerning about the influence on band profiles in single dot, and not treat of the relation of the energy level shift and the dot shape.

In this paper we will focus on the energy level shifts in different shape of semiconductor QD in high strain. We select three shapes of QD to analyze. They are pyramid QD, truncated pyramid QD, and lens QD. By comparing the energy level shifts in these shapes of dots, the difference of the energy level shifts in them are listed, and the relations of the strain and the energy level of QD shape are given.

Starting from the hydrostatic and biaxial components of the strain, the band-edge at the Brillouin zone center ($\vec{k}=0$) can be calculated. In the framework of the eight-band $\vec{k}\cdot\vec{p}$ the energy shifts (conduction-band $\Delta E_{\rm c}$, heavy-hole band $\Delta E_{\rm hh}$, light-hole band $\Delta E_{\rm lh}$, and split-off band $\Delta E_{\rm so}$) are given by[4]

$$\Delta E_{\rm c}=\Delta E_{\rm c}^{hy}=a_{\rm c}\left(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}\right), \tag{1}$$

$$\Delta E_{\rm hh}=a_v\varepsilon_h-\frac{1}{2}\delta E^{\rm sh}, \tag{2}$$

$$\Delta E_{\rm lh}=a_v\varepsilon_h+\Delta E_{\rm lh}^{\rm sh}, \tag{3}$$

$$\Delta E_{\rm so}=a_v\varepsilon_h+\Delta E_{\rm so}^{\rm sh}, \tag{4}$$

where

$$\Delta E_{\rm hh}^{\rm sh}=-\frac{1}{2}\delta E^{\rm sh}, \tag{5}$$

$$\Delta E_{\rm lh}^{\rm sh}=-\frac{1}{2}\Delta_0+\frac{1}{4}\delta E^{\rm sh}+\frac{1}{2}\left[\Delta_0^2+\Delta_0\cdot\delta E^{\rm sh}+\frac{9}{4}\left(\delta E^{\rm sh}\right)^2\right]^{1/2}, \tag{6}$$

$$\Delta E_{\rm lh}^{\rm sh}=-\frac{1}{2}\Delta_0+\frac{1}{4}\delta E^{\rm sh}-\frac{1}{2}\left[\Delta_0^2+\Delta_0\cdot\delta E^{\rm sh}+\frac{9}{4}\left(\delta E^{\rm sh}\right)^2\right]^{1/2}, \tag{7}$$

where Δ_0 is the spin-orbit splitting in the absence of strain. The strain shift $\delta E^{\rm sh}$ depends on the interface orientation. In the case of growth on (001) substrate

$$\delta E^{\rm sh}=b\left(2\varepsilon_{zz}-\varepsilon_{xx}+\varepsilon_{yy}\right), \tag{8}$$

where b is the shear deformation potential. The hydrostatic strain component

$$\varepsilon_h=\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}. \tag{9}$$

In our study, we analyzed the hydrostatic and biaxial strain components in the QD grown on GaAs substrate, with the help of the finite element method. Via Eqs. (1)—(9) the shifts of the band profile are obtained.

The calculations were made under the following conditions: (1) elastic isotropy is assumed in the analysis; (2) the interactions among QD is ignored; (3) the poisson rate we adopted in this paper are E= 51.42 GPa and v = 0.35 respectively for the super cell; (4) the aspect ratio h/a (where a is the QD base and h is its height) in the three shaped quantum dots are the same (select h/a=0.25), The growth direction is along the [001] direction points upward, which means that the QD is growth on the (001) surface of the substrate.

To models the lattice mismatch that is responsible for the island formation, a pseudo thermal expansion of the island and the wetting-layer is applied and which make such section of the material experience a uniform thermal expansion in all directions. The temperature is raised by 1 K, and material thermal expansion coefficient is $|\varepsilon_0|$ (0.067). So the thermal strain is defined as

$$\varepsilon_{\rm T}=\varepsilon_0\Delta T, \tag{10}$$

which is the base of the calculated stain components.

The hydrostatic and biaxial strain components per unite area along the growth direction are shown in Figs. 1 and 2, respectively. The full line, dot line, and dot-dashed line denote the pyramid dot, the truncated pyramid dot, and the lens dot, respectively. From Figs. 1 and 2 we can see that the two stain components are almost constant. Equations (1)—(8) are the substitution for the two strain components. The shifts of every level in the three QDs are shown in Table 1. From Table 1 we can see that when the aspect ratio is fixed, the energy level shifts of the three QDs satisfy the patterns as follows.

For a dot, the energy levels is nondegenerate, and the energy shift is not the same in different bands. Because the shift of the conduction-band ($\Delta E_{\rm c}$) is positive, the conduction-band increases, and so does the shift of heavy-hole band ($\Delta E_{\rm hh}$). In contradiction to the shifts of the light-hole band ($\Delta E_{\rm lh}$) and split-off band ($\Delta E_{\rm so}$) are negative, the two bands decreases.

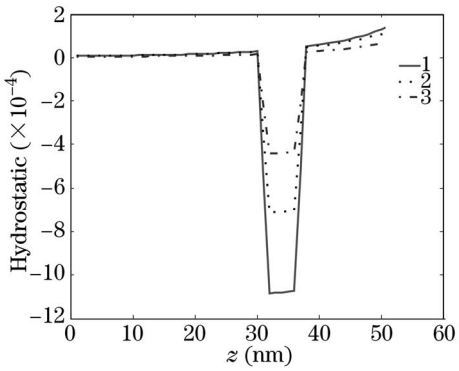

Fig. 1. Hydrostatic strain component per unite area as a function of position along the growth direction.

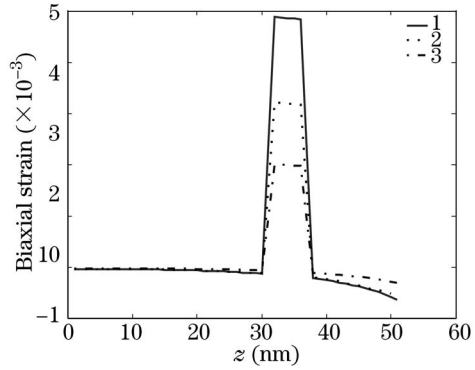

Fig. 2. Biaxial strain component per unite area as a function of position along the growth direction.

Table 1. The Shifts of Every Energy Level in the Three Quantum Dots

	$\Delta E_{\rm c}$ (eV)	$\Delta E_{\rm hh}$ (eV)	$\Delta E_{\rm lh}$ (eV)	$\Delta E_{\rm so}$ (eV)
Pyramid	0.00588	0.0032	−0.1563	−0.2296
Truncated	0.00381	0.0021	−0.1555	−0.2289
Lens	0.00229	0.0012	−0.1549	−0.2283

For a fixed band, the energy shifts is not the same in different dots. The shift of the pyramid dot is the maximum, the lens pyramid dot is the minimum, and the truncated shaped dot is between them. Compared with the value of the band gap band energy, the values of shifts in conductor band and heavy-hole band are small, but the values of the shifts in light-band and split-off band are large. The further can be neglect, the later can not. These changes of energy level will be transformed in the PL spectrum.

These results can be explained by the continuous elastic theory. There is different strain relaxation in different shapes of quantum dots, and thus the elastic energy is not the same[5]. Because of more strain in the pyramid dot, the shift of the energy level is the most.

In conclusion, the shift of energy level is related to the shape of the quantum dot under high strain. The energy level of quantum dot can be influenced by the strain inside it.

This work was supported by the National "863" Project of China (No. 2003AA311070). H. Yang's e-mail address is yhbyddx@sohu.com.

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