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Wetting layers effect on InAs/GaAs quantum dots

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ABSTRACT

FEM combining with the K · P theory is adopted to systematically investigate the effect of wetting layers on the strain-stress profiles and electronic structures of self-organized InAs quantum dot. Four different kinds of quantum dots are introduced at the same height and aspect ratio. We found that 0.5 nm wetting layer is an appropriate thickness for InAs/GaAs quantum dots. Strain shift down about 3%∼4.5% for the cases with WL (0.5 nm) and without WL in four shapes of quantum dots. For band edge energy, wetting layers expand the potential energy gap width. When WL thickness is more than 0.8 nm, the band edge energy profiles cannot vary regularly. The electron energy is affected while for heavy hole this impact on the energy is limited. Wetting layers for the influence of the electronic structure is obviously than the heavy hole. Consequently, the electron probability density function spread from buffer to wetting layer while the center of hole's function moves from QDs internal to wetting layer when introduce WLs. When WLs thickness is larger than 0.8 nm, the electronic structures of quantum dots have changed obviously. This will affect the instrument's performance which relies on the quantum dots' optical properties.

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1. Introduction

In recent years, self-assembled quantum dots, composed by alloy semiconductor such as GeSi, InAs, InSb, have attracted considerable attention for their broad potential application in optoelectronic devices. One of the methods to fabricate self-assembled quantum dots is called the Stranski–Krastanov (SK) epitaxial growth process [1]. During this process, epitaxial layer initially forms a thin epitaxial film known as the wetting layer (WL). In generally, self-assembled quantum dots will lie on this thin layer [2]. Current research shows that, wetting layer plays an important role in the self-organized quantum dots [3]. This layer not only affects the distribution of strain profiles, but also leads to a decrease in the energy gap between the ground state electron and hole energy [4]. Very recently, the effect of WL on electronic structures of truncated-pyramid InAs/GaAs quantum dots has been studied. Analytical continuum strain model and K · P theory are adopted [5].

InAs/GaAs quantum dot, which is a typical Stranski–Krastanov growth model due to its mismatch, has assumed increasing importance in recent years as its application in long-wavelength optoelectronic devices [6]. Many prominent works concentrating on the band energy and electronic structures of InAs/GaAs quantum dots have been accomplished [7]. Unfortunately, WL influence is usually omitted or seldom discussed in the past. Although there have been some works focus on the wetting layer, a complete investigation of the effect of wetting layer on the physical properties of InAs/GaAs quantum dot is still necessary. Thus, the main motivation of this paper is to extend the previous theoretical studies, by systematically investigating the wetting layer's affection on the different shape of InAs/GaAs quantum dot. Four different geometries of InAs/GaAs quantum dots, namely, truncated pyramid, pyramid, truncated-hexagonal and lens, are introduced. The finite element method (FEM) combined with four-band K · P theory are used to calculate strain field and electronic structure of these systems. This paper is organized as follows. Our theoretical model and methods are proposed in Section 2. In Section 3, our results and discussions are listed. And finally, conclusions are given in Section 4.

2. Theoretical model and methods

2.1. Theoretical model

Fig. 1 shows the model established in this paper. The Cartesian coordinate system is used in these models. According to its zinc-blende structure, we take *x*-axis, *y*-axis, *z*-axis for crystal orientation [1 0 0], [0 1 0], [0 0 1], respectively [8].

As presented in Fig. 1, the four kinds of InAs QDs height and base width are 3 nm and 6 nm, respectively. In other words, the

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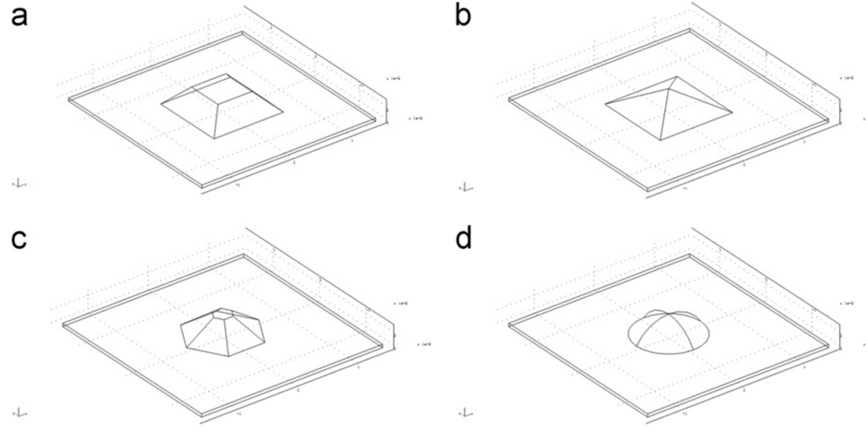

Fig. 1. Configurations of different quantum dots. (a) truncated pyramid; (b) pyramid; (c) truncated hexagonal; and (d) lens.

aspect ratio is kept at 0.5. The GaAs substrate and capping layer dimensions both set to be $30 \times 30 \times 30$ nm.

In order to investigate the effect induced by wetting layer, the layer thickness will set as 0, 0.5, 0.8 and 1.0 nm, respectively.

2.2. Strain and band-edge profile

The anisotropy property is considered in these models. The stiffness matrix is chosen to describe the dependence of the stress component. For an anisotropy sphalerite structure, the stiffness matrix can be written as

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

To obtain the strain and stress, we firstly set the initial strain as

$$\varepsilon_{ij}^0=\begin{cases} \varepsilon_{xx}^0=\varepsilon_{yy}^0=\varepsilon_{zz}^0=\frac{a_{GaAs}-a_{InAs}}{a_{InAs}} \\ \varepsilon_{ij}^0=0, i\neq j \end{cases}, \tag{2}$$

where a_{GaAs}, a_{InAs} are the lattice constants of the substrates and quantum dot, respectively.

Then, we can calculate model's strain distribution after relaxation in three dimensions by using the following equations

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

$$\sigma=\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{zx} \end{pmatrix}=D\cdot(\varepsilon-\varepsilon^0)+\sigma^0 \tag{4}$$

where u, v and w are the compression or expansion misfit of the lattice in the directions of x-, y- and z-axis [9].

According to the K · P theory, we can derive the strain modified band-edge energy. The electron and heavy hole band-edge energy, and the hydrostatic strain can be express as follows:

$$E_{cm}=E_{av}+\frac{\Delta}{3}+E_g+a_c\varepsilon_{hyd} \tag{5}$$

$$E_{hh}=E_{av}+\frac{\Delta}{3}+a_v\varepsilon_{hyd}-\frac{1}{2}b\varepsilon_{bi} \tag{6}$$

$$\varepsilon_{hyd}=\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}. \tag{7}$$

where the bi-axial strain is expressed as $\varepsilon_{bi}=2\varepsilon_{zz}-\varepsilon_{xx}-\varepsilon_{yy}$. In the above equations, a_c, a_v and b is deformation potential of conduction band, deformation potential of valence band and shear deformation potential, respectively. Besides, E_{av} is average valence band energy, E_g is band gap and "Δ" is corresponding to spin-orbital separation energy.

2.3. Electronic structure

To obtain the electron and heavy hole energy, we adapt the four-band K · P theory. The Hamiltonian can be expressed as

$$H=\begin{pmatrix} -(P+Q) & S_- & -R & 0 \\ S_-^\dagger & -(P-Q) & -C & -R \\ -R^\dagger & -C^\dagger & -(P-Q) & -S_+^\dagger \\ 0 & -R^\dagger & -S_+ & -(P+Q) \end{pmatrix} \tag{8}$$

where

$$P=\frac{1}{2m_0}(\hat{p}_x\gamma_1\hat{p}_x+\hat{p}_y\gamma_1\hat{p}_y+\hat{p}_z\gamma_1\hat{p}_z)+P_\varepsilon+V_h \tag{9}$$

$$Q=\frac{1}{2m_0}(\hat{p}_x\gamma_2\hat{p}_x+\hat{p}_y\gamma_2\hat{p}_y-2\hat{p}_z\gamma_2\hat{p}_z)+Q_\varepsilon \tag{10}$$

$$S_\pm=\frac{1}{2m_0}2\sqrt{3}\left[(\hat{p}_x\pm i\hat{p}_y)(\sigma-\delta)\hat{p}_z+\hat{p}_z\pi(\hat{p}_x\pm i\hat{p}_y)\right] \tag{11}$$

$$R=\frac{1}{2m_0}\sqrt{3}\left[(\hat{p}_x+i\hat{p}_y)\mu(\hat{p}_x+i\hat{p}_y)-(\hat{p}_x-i\hat{p}_y)\overline{\gamma}(\hat{p}_x-i\hat{p}_y)\right] \tag{12}$$

$$C=\frac{1}{2m_0}2\left[\hat{p}_z(\sigma-\delta-\pi)(\hat{p}_x-i\hat{p}_y)-(\hat{p}_x-i\hat{p}_y)(\sigma-\delta-\pi)\hat{p}_z\right] \tag{13}$$

$$\sigma-\delta=\frac{1}{6}(-1-\gamma_1+2\gamma_2+6\gamma_3) \tag{14}$$

$$\pi=\frac{1}{6}(1+\gamma_1-2\gamma_2) \tag{15}$$

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