Electronic structures of stacked layers quantum dots: influence of the non-perfect alignment and the applied electric field*

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Electronic structures of the artificial molecule comprising two truncated pyramidal quantum dots vertically coupled and embedded in the matrix are theoretically analysed via the finite element method. When the quantum dots are completely aligned, the electron energy levels decrease with the horizontally applied electric field. However, energy levels may have the maxima at non-zero electric field if the dots are staggered by a distance of several nanometers in the same direction of the electric field. In addition to shifting the energy levels, the electric field can also manipulate the electron wavefunctions confined in the quantum dots, in company with the non-perfect alignment.

Keywords: electronic structure, quantum dot, non-perfect alignment, electric field

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1. Introduction

Nowadays, sophisticated hetero-epitaxial growth technique enables us to obtain various nanostructures on demand. Among them, quantum dots (QDs) may be the best candidates in fabricating optoelectronic devices such as the semiconductor laser,[1−3] the photodetector[4,5] and the single photon source[6,7] due to their three-dimensional quantum confinement for the carriers. In QD lasers, the size uniformity and the vertical alignment of QDs are critical to the performance of the laser. It is expected for experimental researchers to form stacked QDs showing high uniformity within one layer and perfect alignment between adjacent layers.[8,9] As for the theoretician, electronic properties in lateral or vertical coupled QDs are intensively studied[10−13] to give the instruction or prediction on the experiment.

Not only restricted by the quantum confinement, the carriers in QDs are also influenced by the external potential such as the electric field. Stark effect is the signature for the QD placed in the electric field.[14,15] For vertically coupled QDs, on the one hand, the electric field along the growth direction (the z axis) modifies the carrier's wavefunction distribution[16,17] and verifies the growth process of intentionally strongly asymmetric double QDs.[18] On the other hand, the horizontally oriented (in the x–y plane) electric field may be more appealing to researchers in detecting the stagger between the QDs in different layers.[10] Until now, however, it is still impossible to grow QDs without any defects in alignment between layers. Therefore, it is essential to study the electronic and optical properties of staggered QDs to give instructions in analysing the device performance.

In this paper, we calculate electron energy levels in the nanostructure of two vertical coupled QDs grown following the wetting layers. It is found that the energy level curves are asymmetric as the electric field intensity increases from negative to positive in the x axis, along this direction the QDs are apart from each other by several nanometers. Besides the effect on energy levels, the electric field also manipulates the electron wavefunctions in company with the

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non-perfect alignment, leading to the phenomenon of wavefunction localized within only one dot sometimes.

2. Theoretical model

We choose InAs/GaAs QDs that are typical heterostructure in crystal growth and optoelectronic devices. The cross section (the x–z plane) of the computing model is shown in Fig. 1. Placed on the respective 1-nm wetting layer, each InAs QD is truncated pyramidal shape with upper base of 10 nm, bottom base of 16 nm and height of 4 nm. The cases of two QDs being apart from each other with $h = 6$ and 9 nm in the z axis, and with $d = 0$, 3 and 5 nm in the x axis are taken in our calculation.

Before analysing electronic structures, the strain distribution originating from the large lattice mismatch in this system should be considered for its evident modification on both the conduction and valence band edge.[19,20] In continuum elastic theory, the stress can be correlated with the strain by the stiffness matrix, expressed as

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{zx} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \varepsilon_0 \\ \varepsilon_{yy} - \varepsilon_0 \\ \varepsilon_{zz} - \varepsilon_0 \\ \varepsilon_{xy} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \end{pmatrix} + \sigma_0, \tag{1}$$

where σ_0 and ε_0 are the initial stress and strain. The former is set to be zero in both InAs QDs and GaAs barrier; the latter is chosen as the lattice mismatch of the heterostructure, i.e. $\varepsilon_0 = (a_{\mathrm{GaAs}} - a_{\mathrm{InAs}})/a_{\mathrm{InAs}}$ for the QDs and zero for the barrier. The C_{ij} in Eq. (1) means the elastic constants.

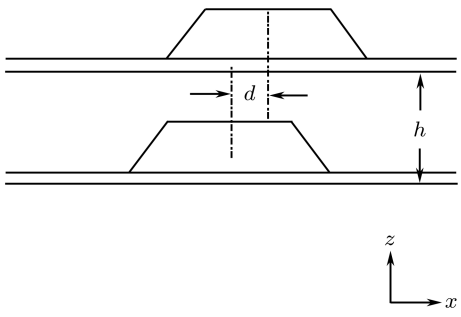


Fig. 1. The cross section of the computing InAs/GaAs QDs model.

The Schrödinger equation governing the electron motion in the QDs with a horizontal electric field is expressed as

$$\begin{aligned} H\Psi &= -\frac{\hbar^2}{2}\nabla \cdot \left(\frac{1}{m^*}\nabla\Psi\right) + (V_0 + V_{\mathrm{strain}} + V_{\mathrm{E}})\,\Psi \\ &= E\Psi. \end{aligned} \tag{2}$$

In Eq. (2), $V_{\mathrm{E}} = -e_0 Ex$ is the potential caused by the horizontal electric field, V_0 is the band offset, and V_{strain} is the band edge modification induced by the strain. For the electron, the expression of V_{strain} is

$$V_{\mathrm{strain}} = a_{\mathrm{c}}\left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}\right), \tag{3}$$

where a_{c} is the conduction band deformation potential. The finite element method (FEM) is adopted to calculate electronic structures of the QDs for its successful application in nanostructures.[21–27] The material parameters used in our calculation are taken from Ref. [28] and we assume the valence band edge of the bulk GaAs as the zero potential point.

3. Results and discussion

First, the dependence of the electron energy levels on the horizontal electric field (along the x axis) is shown in Fig. 2, with different h and d of the QDs. The relationships between energy levels and the electric field intensity in Fig. 2(a) ($h = 6$ nm, $d = 0$ nm) and (d) ($h = 9$ nm, $d = 0$ nm) are symmetric about 0 kV/cm. This is reasonable because the perfectly vertical alignment of the QDs, there is no difference for the electric field either along the positive or along the negative direction of the x axis. Moreover, larger h increases energies of the ground, the second and the third excited states; however, it has little effect on the first excited state.

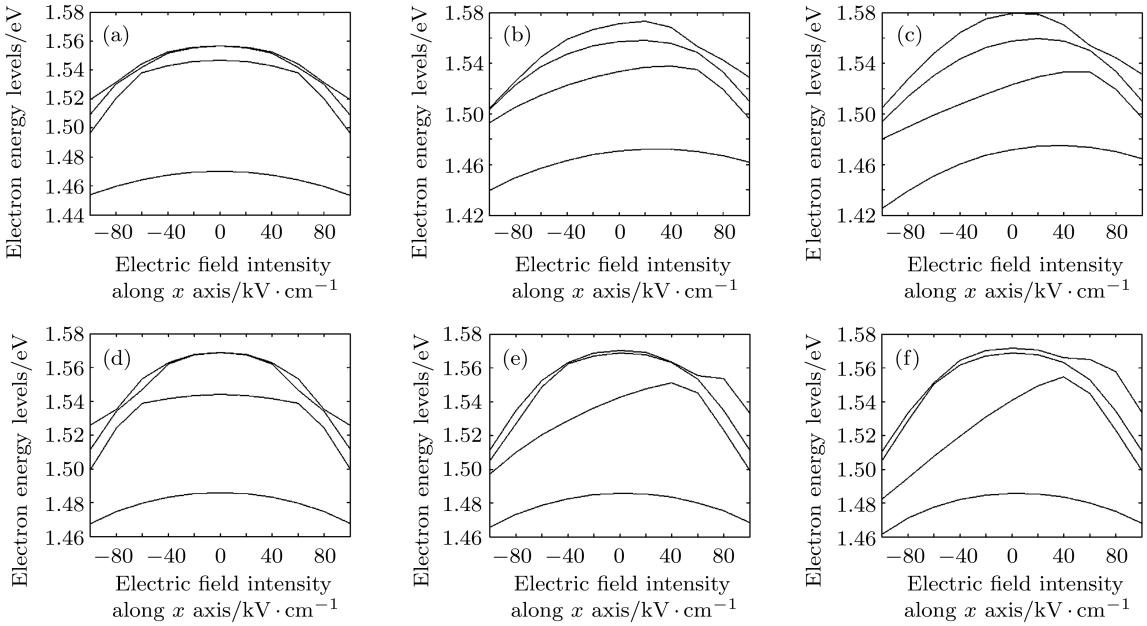


Fig. 2. The dependence of the electron energy levels on the horizontal electric field (along the x axis) with (a) $h = 6$ nm, $d = 0$ nm; (b) $h = 6$ nm, $d = 3$ nm; (c) $h = 6$ nm, $d = 5$ nm; (d) $h = 9$ nm, $d = 0$ nm; (e) $h = 9$ nm, $d = 3$ nm; (f) $h = 9$ nm, $d = 5$ nm of the QDs.

If we move the upper dot several nanometers along the x axis, the energy levels versus the electric field intensity are more interesting, as shown in Figs. 2(b), 2(c), 2(e) and 2(f). Comparing Figs. 2(b) ($h = 6$ nm, $d = 3$ nm) and 2(e) ($h = 9$ nm, $d = 3$ nm), and comparing Figs. 2(c) ($h = 6$ nm, $d = 5$ nm) and 2(f) ($h = 9$ nm, $d = 5$ nm), it is found that larger h reduces the asymmetry of the ground and the second excited state energy levels induced by the horizontal electric field. The first excited state energy is more asymmetric than other levels, exhibiting the maximum at 60 kV/cm for $h = 6$ nm (Figs. 2(b) and 2(c)) and 40 kV/cm for $h = 9$ nm (Figs. 2(e) and 2(f)). In Figs. 2(b) and 2(c), the non-perfect alignment of the QDs dispels the degeneracy between the second and the third excited states under weak electric field shown in Fig. 2(a). But the degeneracy under weak electric field shown in Fig. 2(d) almost keeps the same as shown in Figs. 2(e) and 2(f).

Next, we will analyse the influence of the non-perfect alignment and the applied electric field on the localization of the electron wavefunction. Figure 3 shows the ground state and the first excited state electron wavefunctions in the cross section (the x–z plane) of the QDs, with the horizontal electric field intensities of $E = 0$ (Figs. 3(a) and 3(b)) and $E = 50$ kV/cm (Figs. 3(c) and 3(d)). The geometric parameters are $d = 0$ nm and $h = 6$ nm. The ground state electron is trapped in the lower dot with higher probability because the strain-induced modification of the conduction band edges (Figs. 3(a) and 3(c)). The electric field shifts the wavefunctions evidently. For the first excited state, the wavefunction fraction in the lower dot is more influenced by the field (Fig. 3(d)).

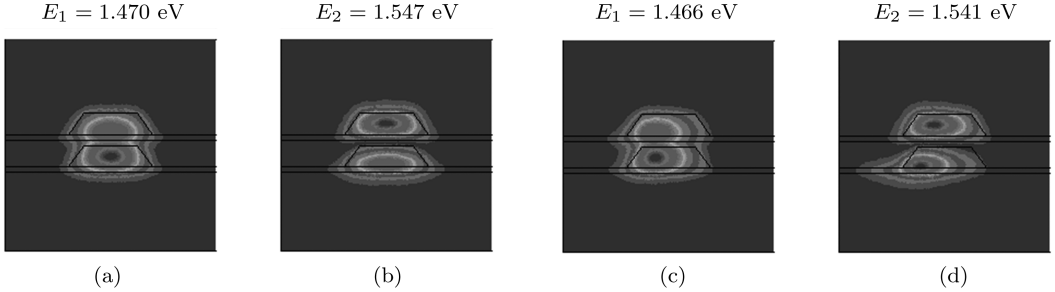


Fig. 3. The electron wavefunctions of the QDs with $d = 0$ and $h = 6$ nm: (a) ground state, $E = 0$; (b) first excited state, $E = 0$; (c) ground state, $E = 50$ kV/cm; and (d) first excited state, $E = 50$ kV/cm.

Figure 4 depicts the ground state and the first excited state electron wavefunctions in the cross section of the staggered QDs, with the horizontal electric field intensity $E = 0$ (Figs. 4(a) and 4(b)) and $E = 50$ kV/cm (Figs. 4(c) and 4(d)). The geometric parameters are $d = 3$ and $h = 6$ nm here. Without the electric field, the first excited wavefunction tends to be localized in the staggered QDs' corner, as shown in Fig. 4(b). However, the first excited wavefunction fraction in the upper dot returns to the middle position under the electric field, as shown in Fig. 4(d).

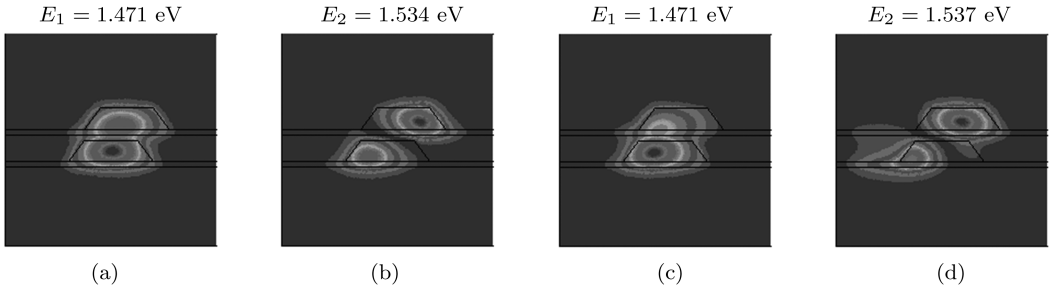


Fig. 4. The electron wavefunctions of the staggered QDs with $d = 3$ nm and $h = 6$ nm: (a) ground state, $E = 0$; (b) first excited state, $E = 0$; (c) ground state, $E = 50$ kV/cm; and (d) first excited state, $E = 50$ kV/cm.

Figure 5 depicts the electron wavefunctions in the staggered QDs of $d = 5$ nm and $h = 9$ nm, under the horizontal electric field intensity $E = 0$ (Figs. 5(a) and 5(b)) and $E = 50$ kV/cm (Figs. 5(c) and 5(d)). When there is no electric field, the wavefunction of the ground state is mainly localized in the lower dot but the wavefunction of the first excited state is mainly localized in the upper dot. This is similar to the cases in Figs. 3 and 4. Here the attraction is the wavefunction under the electric field. The ground state or the first excited state wavefunction only appears in the lower or upper dot, respectively.

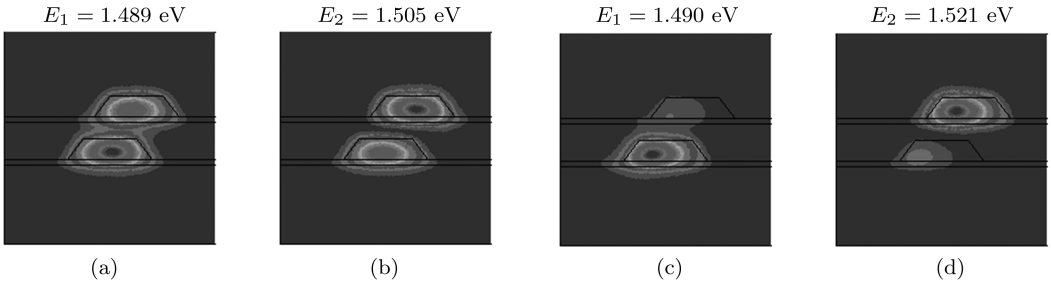


Fig. 5. The electron wavefunctions of the staggered QDs with $d = 5$ nm and $h = 9$ nm: (a) ground state, $E = 0$; (b) first excited state, $E = 0$; (c) ground state, $E = 50$ kV/cm; and (d) first excited state, $E = 50$ kV/cm.

4. Summary

Electronic structures of double stacked QDs are theoretically studied by using the FEM. The dependence of electronic structures on the non-perfectly vertical alignment of QDs and the applied electric field are analysed. The relationship between the electron energy levels and the horizontal electric field provides an effective method to estimate whether the QDs are perfectly aligned. In the staggered QDs, it is possible to trap the electron in only one dot by adjusting the vertical and horizontal distances of the QDs and the electric field intensity. Our results are helpful in studying the growth of the stacked layers of QDs and fabricating the optoelectronic devices.

References

[1] Huffaker D L, Park G, Zou Z, Shchekin O B and Deppe D G 1998 *Appl. Phys. Lett.* **73** 2566

[2] Wang Z G, Chen Y H, Liu F Q and Xu B 2001 *J. Cryst. Growth* **227** 1132

[3] Sellin R L, Ribbat C, Bimberg D, Rinner F, Konstanzer

H, Kelemen M T and Mikulla M 2002 *Electron. Lett.* **38** 883

[4] Chu L, Zrenner A, Bohm G and Abstreiter G 1999 *Appl. Phys. Lett.* **75** 3599

[5] Chen S D, Chen Y Y and Lee S C 2005 *Appl. Phys. Lett.* **86** 253104

[6] Michler P, Kiraz A, Becher C, Schoenfeld W V, Petroff P M, Zhang L D, Hu E and Imamoğlu A 2000 *Science* **290** 2282

[7] Pelton M, Santori C, Vučković J, Zhang B Y, Solomon G S, Plant J and Yamamoto Y 2002 *Phys. Rev. Lett.* **89** 233602

[8] Ledentsov N N, Shchukin V A, Grundmann M, Kirstaedter N, Böhrer J, Schmidt O, Bimberg D, Ustinov V M, Egorov A Y, Zhukov A E, Kop'ev P S, Zaisev S V, Gordeev N Y, Alferov Z I, Borovkov A I, Kosogov A O, Ruvimov S S, Werner P, Gösele U and Heydenreich J 1996 *Phys. Rev.* B **54** 8743

[9] Pei Q X, Lu C and Wang Y Y 2003 *J. Appl. Phys.* **93** 1487

[10] Szafran B, Peeters F M and Bednarek S 2007 *Phys. Rev.* B **75** 115303

[11] Terzis A F, Kosionis S G and Paspalakis E 2007 *J. Phys.* B **40** S331

[12] Persano A, Cola A, Taurino A, Catalano M, Lomascolo M, Convertino A, Leo G, Cerri L, Vasanelli A and Vasanelli L 2007 *J. Appl. Phys.* **102** 094314

[13] Voskoboynikov O 2008 *Phys. Rev.* B **78** 113310

[14] Li S S and Xia J B 2005 *Appl. Phys. Lett.* **87** 043102

[15] Billaud B, Picco M and Truong T T 2009 *J. Phys.*: *Condens. Matter* **21** 395302

[16] Krenner H J, Sabahtil M, Clark E C, Kress A, Schuh D, Bichler M, Absteiter G and Finley J J 2005 *Phys. Rev. Lett.* **94** 057402

[17] Stinaff E A, Scheibner M, Bracker A S, Pomonarev I V, Korenev V L, Ware M E, Doty M F, Reinecke T L and Gammon D 2005 *Science* **311** 636

[18] Bracker A S, Scheibner M, Doty M F, Stinaff E A, Pomonarev I V, Kim J C, Whitman L J, Reinecke T L and Gammon D 2006 *Appl. Phys. Lett.* **89** 233110

[19] Liu Y M, Yu Z Y and Ren X M 2009 *Chin. Phys.* B **18** 16

[20] Califano M and Harrison P 2002 *J. Appl. Phys.* **91** 389

[21] Ye H, Lu P F, Yu Z Y, Song Y X, Wang D L and Wang S M 2009 *Nano Lett.* **9** 1921

[22] Liu Y M, Yu Z Y, Jia B Y, Xu Z H, Yao W J, Chen Z H, Lu P F and Han L H 2009 *Chin. Phys.* B **18** 4667

[23] Gatti R, Marzegalli A, Zinovyev V A, Montalenti F and Miglio L 2008 *Phys. Rev.* B **78** 184104

[24] Belytschko T, Gracie R and Ventura G 2009 *Modelling Simul. Mater. Sci. Eng.* **17** 043001

[25] Ye H, Lu P F, Yu Z Y, Yao W J, Chen Z H, Jia B Y and Liu Y M 2010 *Chin. Phys.* B **19** 047302

[26] Zhao W, Yu Z Y and Liu Y M 2010 *Chin. Phys.* B **19** 067302

[27] Yao W J, Yu Z Y and Liu Y M 2010 *Chin. Phys.* B **19** 077101

[28] Vurgaftman I, Meyer J R and Ram-Mohan L R 2001 *J. Appl. Phys.* **89** 5815