Analysis of Wetting Layer Effect on Electronic Structures of Truncated-pyramid Quantum Dots

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***Abstract*—A theoretical analysis of wetting layer effect on electronic structures of InAs/GaAs truncated-pyramid quantum dots is carried out using an eight-band Fourier transform-based k•p method. Wetting layer changes ground-state energy significantly whereas modifies probability density function only a little. The main acting region of wetting layer is just underneath the base of the dot.**

I. INTRODUCTION

Self-assembled quantum dots in the application of optoelectronics are usually fabricated by the Stranski-Krastanov (SK) epitaxial growth model [1]. Taking the structure shown in Fig.1 as an example, about a 1-2ML InAs wetting layer (WL) is grown on a substrate, followed by a spontaneous coherent InAs island formation process. Finally, a deposition of an additional GaAs material, which is usually the same material as the substrate, is adopted to cover the quantum-dot island. WL does play a quantum-well effect on the strain distribution and electronic structures of quantum dots. However, they are usually omitted or seldom discussed by considering the very thin thickness of the WL in the past works [2]-[4]. Therefore, it is necessary to examine the effect of WL completely, especially for those structures with high aspect ratios. S. Lee *et al*. [5] have investigated the effect of WL on properties of lens-shape quantum dots using the combination of an atomic strain model and the empirical tight-banding model that are much complicated than the combination of a continuum strain model and the k•p model. Consequently, we adopt an eight-band Fourier transform-based k•p method [6]-[7] together with an analytical continuum strain model [3] to study effect of WL on electronic structures of truncated-pyramid quantum dots in this article. We first investigate effect of WL on ground-state energies of quantum dots with different heights, and then we adopt half-truncated structures to find the detail information of WL effect.

II. COMPUTATION METHODS

Electronic structures of quantum dots are usually obtained by solving equation including envelop function F(r) and position-dependent Hamiltonian matrix H(r;k) with differential operators,

$$\mathbf{H}\left(\mathbf{r};\hat{k}_x,\hat{k}_y,\hat{k}_z\right)\mathbf{F}(r)=E\mathbf{F}(\mathbf{r}), \tag{1}$$

where E is the energy.

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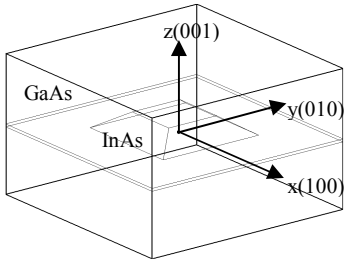

Fig. 1 Geometric model of a truncated-pyramid InAs/GaAs quantum-dot structure. The bottom dimension, the top dimension, and the height of dot are 12nm, 12*f* nm, and 6(1-f) nm, respectively. The thickness of WL is 0.5nm. *f* is the truncation factor.

Envelop function F(r) can be approximated using Fourier series and complex exponential components, and the Fourier transform of the spatially-varying Hamiltonian H(r;k) can be obtained by entering analytical Fourier transform of quantum dot shape functions into the Hamiltonian matrix H(r;k). Therefore, the matrix of Fourier domain Hamiltonian **M** for the eigen-problem can be formulated by a bra-ket operation to (1) utilizing the orthogonality of complex exponential function in F(r), and the new eigen-problem can be written as [6]-[7],

$$[\mathbf{M}_{st}][\mathbf{c}_t]=E[\mathbf{c}_t], \tag{2}$$

where **M** is constructed with Fourier series of H(r;k), and the dimension of **M** is only determined by the order of Fourier frequencies of H(r;k), $\mathbf{c}_t$ is the Fourier series of F(r).

III. RESULTS AND DISCUSSIONS

In this section, we first discuss the influence of WL on ground-state energies of the structure shown in Fig.1 with different truncation factors (*f*=0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9). To make a clear illustration, we also calculate ground-state energies of the dot (structure without WL) shown in Fig.1 with same truncation factors. Fig. 2 shows ground-state energies of electron (E1) and heavy-hole (HH1) of dots with (solid lines) and without (dashed lines) WL under different truncation factors. It can be seen that the difference between the case with WL and the case without WL is obvious only at higher truncation (f≥0.5), especially for HH1. That is to say, significant WL effect only appears when the thickness of WL is comparable with the height of the dot.

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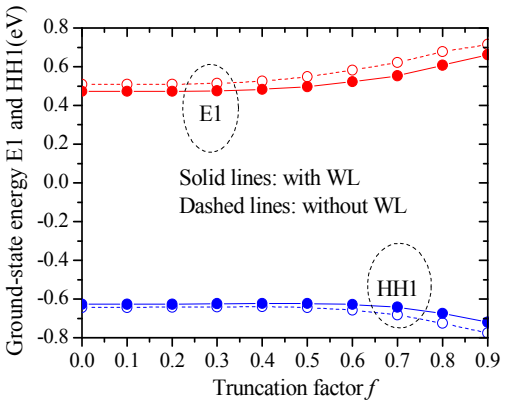

Fig. 2 Ground-state energies E1 and HH1 of a series of truncated-pyramid InAs/GaAs dots with and without inclusion of WL

To further investigate the detail information about effect of WL, we calculate ground-state energy of the half-truncated dot (f=0.5) with a cube just underneath its bottom (denoted as QDC). The thickness of cube is also 0.5nm. Ground-state energy E1 and HH1 of QDC are tabulated in Table I with those of half-truncated structure shown in Fig.1 (denoted as QDW) and half-truncated dot (denoted as QD). Band-edge profiles of QD (dashed lines) and QDW (solid lines) along [001] direction after strain modification are shown in Fig. 3. WL widens potential wells but keeps positions of band edges unchanged almost inside the dot region. As a result, ground-state energy of QDW in Table I varies a lot, especially for ground-state energy of electron owing to the smaller electron mass.

Additionally, it can be seen that discrepancy of ground-state energy between QD and QDW is much more than that between QDW and QDC. This indicates that the main influence of WL on ground-state energy comes from the area just beneath the bottom of the dot. Fig. 3 describes probability density functions (PDFs) corresponding to E1 of QD and QDW. After the action of WL, the center of the PDF of QDW shifts towards the WL region and a very small portion of PDF in the barrier region moves into the region just beneath the bottom of the dot but not the whole WL region. Consequently, effect of WL to electronic structures mainly comes from the region just beneath the bottom of the dot.

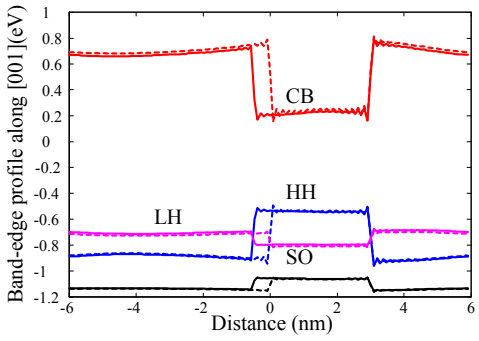

Fig. 3 Band-edge profiles of QD (dashed lines) and QDW (solid lines) along [001] direction.

TABLE 1 GOUND-STATE ENERGY E1, HH1 AND GOUND-STATE ENERGY GAPS Eg OF QD, QDW AND QDC

Ground–state energy	Structures in Calculation		
	QD	QDC	QDW
E1(eV)	0.5472	0.5099	0.4972
HH1(eV)	-0.6437	-0.6308	-0.6223

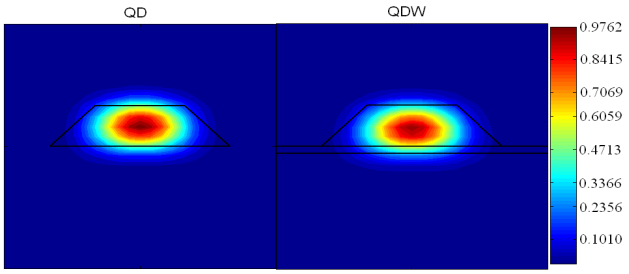

Fig. 4 PDF corresponding to ground-state energy E1 of QD and QDW. The black lines make up the shape section of QD and QDW.

IV. CONCLUSIONS

In summary, we have adopted a continuum strain model and an eight-band Fourier transform-based k•p method to investigate the WL effect on electronic structures of the truncated-pyramid InAs/GaAs quantum dots. WL effect becomes obvious only as the thickness of WL is comparable with the height of the dot. For the half-truncated structure, confinement of WL changes the ground-state energy up to 0.5eV but only drives a small portion of PDF of conduction band from barrier region into WL. WL layers also widens the potential well and thus reduce the energy band-gap, the main influence of WL to electronic structures is just from the region underneath the bottom of the truncated-pyramid dot.

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