Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials, Tokyo, 2004, pp. 616-617

P9-3

Transition Energies in Vertically Coupled Multilayer Nanoscale InAs/GaAs Semiconductor Quantum Dots with Different Structure Shapes

Yiming Li

Department of Computational Nanoelectronics, National Nano Device Laboratories
Microelectronics and Information Systems Research Center, National Chiao Tung University
Address: P.O. BOX 25-178, Hsinchu City, Hsinchu 300, TAIWAN; E-mail: ymli@mail.nctu.edu.tw

1. Introduction

Nanoscale semiconductor quantum dots have recently been of great interest and successive study from different points of view [1-4]. Advanced fabrication technology has been applied to consider another degree of freedom along the growth direction for vertically coupled quantum dots (VCQDs). Evident physical properties in such system are the effect of dot-to-dot interactions on the electronic structure, the electronic entanglement, and the charge transfer [2]. Many studies have considered two-dimensional (2D) lateral geometry and confinement potential to explore the electronic structure of VC 2-layers QDs [2,3]. For the structure with different shapes, 3D modeling is important to clarify the electronic structure of VC multilayers QDs (VCMQDs) under applied magnetic fields **B**.

In this paper, the electronic structure of VCMQDs with different shapes under applied **B** is explored by using a unified 3D model. Our Hamiltonian considers the position- and energy-dependent quasi-particle effective mass approximation and Landé factor, the finite hard wall confinement potential, and the Ben Daniel-Duke boundary conditions. A nonlinear iterative method is applied to solve the 3D VCMQDs' problem with disk (DI), elliptical (EL), and conical (CO) shapes. For the VCMQDs with small QDs at **B** = 0 T, the transition energy is dominated by the number of stacked layers *N*. The inter-distance *d* among QDs plays a crucial role in the tunable states of VCMQDs. For DI-shaped VCMQDs with *d* = 1 nm, variations of the ground and first excited state electron energies are all larger than 30%. Under **B**, the energy band gap of VCMQDs shifts with the strength of **B** and becomes wake when *N* increases. This study is constructive in studying the magneto-optical phenomena and quantum optical structures.

2. A Three-Dimensional Computational Model

As shown in Fig. 1, for VCMQDs in the one-band envelope-function formalism, effective Hamiltonian is

$$\hat{H} = \boldsymbol{\Pi}_{\mathbf{r}} \frac{1}{2m(E,\mathbf{r})} \boldsymbol{\Pi}_{\mathbf{r}} + V(\mathbf{r}) + \frac{1}{2} g(E,\mathbf{r}) \mu_B \mathbf{B}\boldsymbol{\sigma}, \quad (1)$$

where $\boldsymbol{\Pi}_{\mathbf{r}}$ is the electron momentum vector. $m(E,\boldsymbol{r})$ and $g(E,\boldsymbol{r})$ are the electron effective mass and Landé factor

$$\frac{1}{m(E,\mathbf{r})} = \frac{2P^2}{3\hbar^2}\left[\frac{2}{E - E_g(\mathbf{r}) - V(\mathbf{r})} + \frac{1}{E - E_g(\mathbf{r}) - V(\mathbf{r}) + \Delta(\mathbf{r})}\right] \text{ and } \quad (2)$$

$$g(E,\mathbf{r}) = 2\left\{1 - \frac{m_0}{m(E,\mathbf{r})} \frac{\Delta(\mathbf{r})}{3(E + E_g(\mathbf{r})) + 2\Delta(\mathbf{r})}\right\}. \quad (3)$$

$V(\boldsymbol{r})$ is the confinement potential, $E_g(\boldsymbol{r})$ and $\Delta(\boldsymbol{r})$ are the band gap and spin-orbit splitting in the valence band, P is the momentum matrix element, $\boldsymbol{\sigma}$ is the vector of the Pauli matrix. The Ben Daniel-Duke boundary condition for the wavefunction $\Psi(\mathbf{r})$ between material interface $\mathbf{r}_s$ is

$$\Psi_1(\mathbf{r}_s) = \Psi_2(\mathbf{r}_s) \text{ and } \left\{\frac{\hbar^2}{2m(E,\mathbf{r})} \nabla_{\mathbf{r}}\right\}_n \Psi(\mathbf{r}_s) = const. \quad (4)$$

To solve the corresponding multi-dimensional nonlinear Schrödinger equation derived from (1)-(4), the nonlinear iterative method [4] has been generalized to compute the "self-consistent" solution of the problem.

3. Results and Discussion

A 10-layers vertically stacked QDs system is studied, where InAs dots are embedded into GaAs matrix. Shown in Fig. 1, DI-, EL-, and CO-shaped quantum dot layers are separated by *d* among QD layers. For the VCMQDs with small QDs (e.g., z_0 = 2-4 nm and R_0 = 5-20 nm) separated by a fixed *d*, the transition energy of 10-layers VCMQDs with 3 different shapes is significantly dominated by *N*. When *N* increases the electron transition energy decreases monotonically and eventually tends to a saturated value for $N > 6$. Figs. 2 and 4 show the calculated transition energies versus *N* for the states l = 0 and l = -1. DI- EL, and CO-shaped QDs are with R_0 / z_0 = 10 nm / 2 nm. For the DI-shaped 10-layers VCMQDs with *d* = 1 nm, the electron energy difference is 0.18 eV and its variation is up to 40% for the state of l = 0. The energy transition for l = -1 in DI, EL, and CO shapes is less dependent on *N*. Shown in Figs. 3 and 5, the calculated electron occupancy ratio *W* increases when *N* increases and tends to a saturated value. This confirms the dependence of shapes and *N* on transition energy of the 10-layers VCMQDs. Under **B** = 0 T, Table I summarizes the energy variation for the 10-layers VCMQDs with different shape and *d*. With the similar 3D modeling and simulation, we have calculated the hole energy and for different shapes. The transition energy among the states and the structure's energy band gap are calculated systematically as a function of **B** with arbitrary strength. The calculations of the energy band gap for the 10-layers VCMQDs with different shapes are shown in Figs. 6, 7, and 8, respectively. We observed that the dependence of magnetic fields on the transition energy is reduced when *N* is increased. To verify the calculated transition energies of the stacked QDs quantitatively, transition energies can be measured experimentally from the photoluminescence spectra. This study is useful for the study of quantum optical structures and design of advanced semiconductor photonic and electronic devices.

4. Conclusions

In conclusion, we have presented a unified 3D modeling and simulation for VCMQDs under applied magnetic fields with different shapes and inter-distances among QDs. For small QDs, our examination has shown that the transition energy is directly dominated by the number of stacked layers. The inter-distance among layers also plays a crucial role in the tunable states of the dots. The dependence of magnetic fields on the electron transition energy was depressed when the number of vertically coupled layers is increased.

Acknowledgements

This work is supported in part by the National Science Council (NSC) of TAIWAN under contract No.: NSC – 92 – 2112 – M – 429 – 001 and the grant of the Ministry of Economic Affairs, Taiwan under contract No. 92 – EC – 17 – A – 07 - S1 – 0011.

References

[1] H. Akinaga and H. Ohno, IEEE Trans. Nanotech. **1** (2002) 19; M. Bayer *et al*., Science **291** (2001) 451; D. Bimberg *et al*., Thin Solid Films **367** (2000) 235; A. D. Yoffe, Advances in

Physics **50** (2001) 1.
[2] X. Hu and S. Das Sarma, Phys. Rev. A **61** (2000) 062301; P. Yu *et al*., Phys. Rev. B **60** (1999) 16 680; Y. Tokura *et al*., J. Phys.: Condens. Matter **11** (1999) 6023.
[3] R. Heitz *et al*., Phys. Rev. B **57** (1998) 9050; B. Partoens *et al*., Phys. Rev. Lett. **79** (1997) 3990.
[4] Y. Li *et al*., Comput. Phys. Commun. **147** (2002) 209; Y. Li *et al*., Proc. IEEE-NANO **2** (2003) 99; Y. Li *et al*., Jpn. J. App. Phys. **41** (2002) 2698; Jpn. J. App. Phys. **43** (2004) 2104.

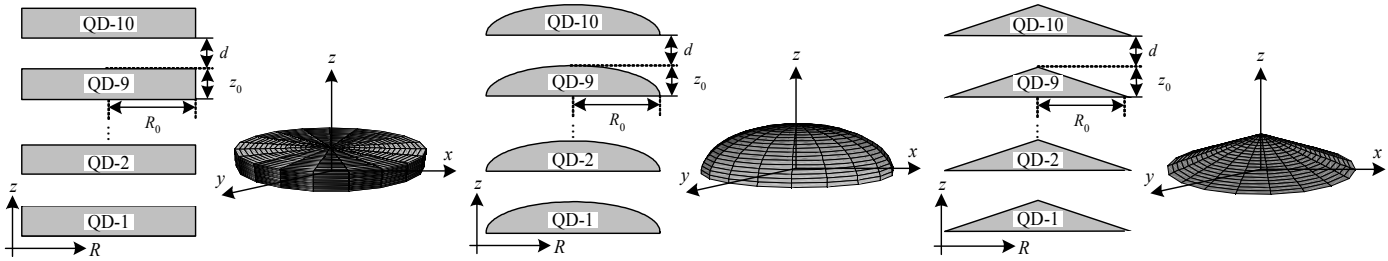

Fig. 1 A 10-layers VCMQDs with DI- (the left figure), EL, and CO-shaped (the right one) QDs. For VCMQDs with small QDs, the d = 1~30 nm, the height z_0 = 1~5 nm, the radius R_0 = 5~20 nm, and N = 2~30. In our study, R_0 / z_0 = 10 nm / 2 nm

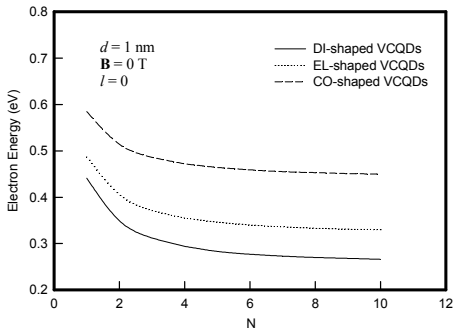

Fig. 2 Electron energy (l = 0) vs. N for the 10-layers VCMQDs under **B** = 0 T with different shapes.

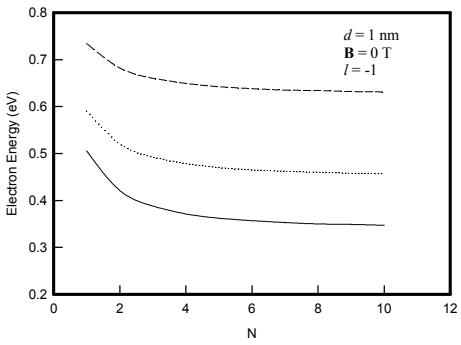

Fig. 4 Electron energy (l = -1) vs. N for the 10-layers VCMQDs under **B** = 0 T with different shapes.

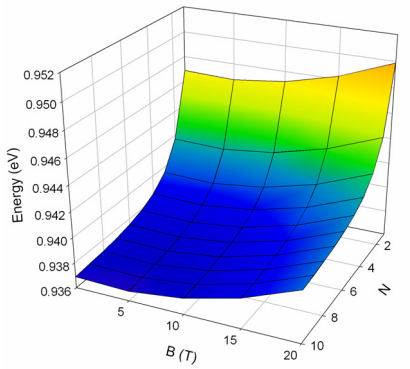

Fig. 6 The energy gap versus N and **B** for the 10-layers InAs/GaAs VCMQDs with DI-shaped QDs , where d = 5 nm.

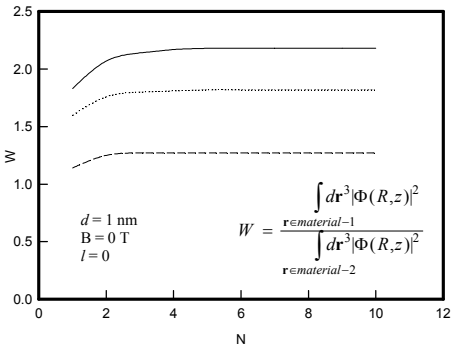

Fig. 3 W vs. N for the 10-layers VCMQDs under **B** = 0 T with different shapes and l = 0.

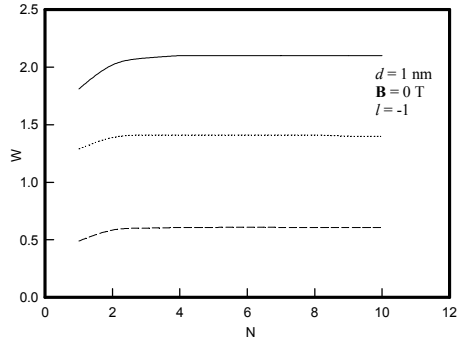

Fig. 5 W vs. N for the 10-layers VCMQDs under **B** = 0 T with different shapes and l = -1.

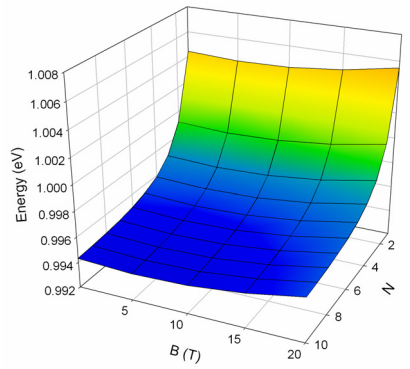

Fig. 7 The energy gap versus N and **B** for the 10-layers InAs/GaAs VCMQDs with EL-shaped QDs , where d = 5 nm.

Table I Electron energy variation of the 10-layers InAs/GaAs VCMQDs at **B** = 0 T with various d. The structure is with DI, EL, and CO shapes, where l = 0 or -1. Electron energy variation is calculated with ($E_{N=1}$ - $E_{N=10}$) / $E_{N=1}$ (%)

	d (nm)	0.5	1	2	3	5
DI shape	l = 0	58.79	39.74	19.28	9.51	2.33
	l = -1	46.26	31.28	15.12	7.40	1.78
EL shape	l = 0	47.11	32.32	16.10	8.15	2.12
	l = -1	32.81	22.71	11.54	5.98	1.65
CO shape	l = 0	32.83	23.04	12.13	6.59	2.02
	l = -1	19.37	14.04	8.04	4.88	2.00

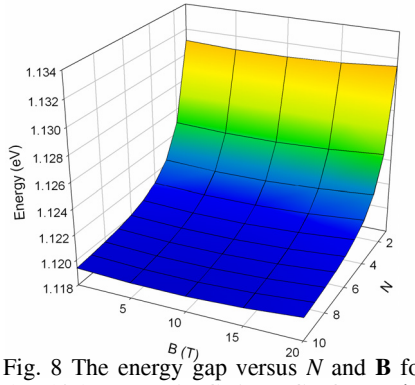

Fig. 8 The energy gap versus N and **B** for the 10-layers InAs/GaAs VCMQDs with CO-shaped QDs , where d = 5 nm.