Journal of New Technology and Materials
JNTM
Vol. 01, N°00 (2011)55-58

OEB Univ. Publish. Co.

Electronic structure calculation of the GaAs/AlAs quantum dot superlattices

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Received: 23 May 2011, accepted: 30 September 2011

Abstract

Theoretical investigation of the electronic structure of GaAs/AlAs quantum dots superlattices is presented. We use the envelope function approximation in connection with Kronig-Penney model to calculate the conduction band structure of the cubic quantum dot crystal. . We show that, when quantum dots are separated by a finite barrier and positioned very close to each other so that there is a significant wave function overlap, the discrete energy levels split into three-dimensional minibands. We can control the electronic structure of this artificial quantum dot crystal by changing theirs technological parameters, the size of quantum dots, interdot distances, barrier height, and regimentation. This type of structure provides electronic and optical properties very important that are different to that of bulk and quantum well superlattices. The proposed engineering of three-dimensional minibands in quantum dot crystals allows one to fine-tune electronic and optical properties of such nanostructures.

Keywords: *quantum dots, semiconductor superlattices, envelope function approximation*

1. Introduction

Recently low dimensional systems at nanometer scale have stimulated a new promising research in condensed matter. Mainly these structures opened a crossover between the physics of bulk condensed matter and few body systems. The progress of experimental techniques have made feasible the possibility of quantum confinement of only few electrons, often referred as "man made structures" [1]. In particular, semiconductor quantum dots (QD) have many potential applications in various domains such in electronic devices, information processing and non-linear optic.

Nanometer-sized semiconductor quantum dots can be grown in the Stranski-Krastanow mode using molecular beam epitaxy [2] or metal-organic chemical vapor deposition [3].

The interest in quantum dot superlattices (QDS) structures combined system lies on the ability to tune optical transition energies by varying SL period as well as by changing QD parameters. Nowadays, the suitability of mid-infrared photodetectors was confirmed [4,5].

In addition, it was shown that QDS together with their wetting layer modify significantly the energy structure in the case of GaAs/AlAs Therefore, in order to determine optimal design for applied purposes, an appropriate knowledge about their optical properties and electronic structures of combined QD/SL systems is fundamental.

The aim of this paper is to investigate the electron energy band structure in a 3D *regimented* array of QD semiconductors by means the envelope function approximation. The regimentation, namely spatial site correlation, along the three directions results in the grow of an artificial crystal, where quantum dots play the role of atoms. Such structure is then referred as a *quantum dot crystal* (QDC). As originally considered by [6], we paid our attention on simple cubic QDC consisting in very small (size about of 5–10 nm) GaAs quantum dots grown on AlAs and surrounded by AlAs cap layer.

In the next section, we outline the theoretical formalism used for calculating 3D energy minibands. It is followed by Section. III, which presents results of the numerical simulation and discussion. Our conclusions are given in Sec. IV.

2. Analytical study

In order to simplify our analytical calculation, we restrict our analysis to simple structures formed by the periodic arrangement of cubic quantum dot, along the three axes x, y and z as shown in Fig (1.a). We also show in this figure the notations used throughout the rest of the article. Our goal in this section is develop a simple, almost analytical, formalism using the envelope function approximation, for carrier transport in QDC that would serve as a useful tool for experimentalists and materials growers.

Theoretical models for quantum dots within the envelope function approximation usually lead to a complex multidimensional Schrödinger equation, which needs to be solved using finite elements method, or plane wave expansion. Application of the pseudopotential methods for QDC is computationally challenging.

In our analyzis, we intersent to the conduction band of the GaAs/AlAs QDC. We this is done for several reasons. First of all, the most of the band gap discontinuity between GaAs and AlAs goes to the conduction band. Second, the potential energy minimum in the conduction band is located in Γ point, which greatly simplifies the model and justifies our omission of carrier Bloch functions from consideration [7].

The Schrödinger equation that describes the motion of a single electron in such a system can be written in the following form:

$$\left[-\frac{\hbar^2}{2}\nabla_r \frac{1}{m^*(r)}\nabla_r + V(r)\right]F(r) = EF(r) \qquad (1)$$

Here, the atomic structure of the host semiconductor enters the analysis as an effective mass m^*. This parameter assumes different values in the quantum dot and the barriers.

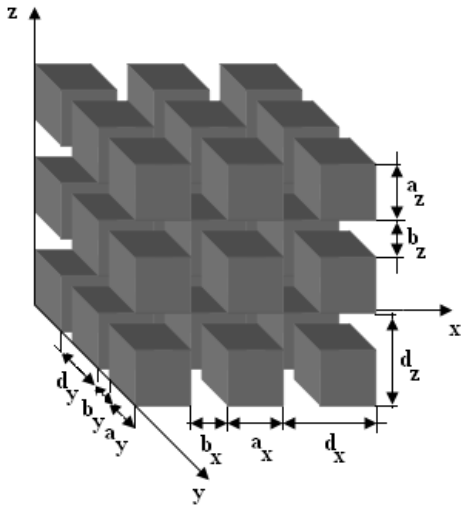

FIG.1. Schematic structure of the cubic QDC

The potential $V(r)$ corresponds to an infinite sequence of quantum dots of size, a_x, a_y and a_z separated by the barriers of thickness, b_x, b_y and b_z. We assume that it is written as a sum of three independent periodic functions of coordinates, x, y and z with periods of d_x, d_y and d_z

$$V(r) = V_x(x) + V_y(y) + V_z(z) \qquad (2)$$

where

$$V_\xi(\xi) = 0 \quad \text{For} \quad \left|\xi - \eta_\xi d_\xi\right| \le a_\xi / 2 \qquad (3)$$

$$V_\xi(\xi) = V_0 \quad \text{For} \quad \left|\xi - \eta_\xi d_\xi\right| \ge a_\xi / 2$$

with $$d_\xi = a_\xi + b_\xi \qquad (4)$$

Here η_ξ are the integer numbers and subscript ξ denotes a particular coordinate axis. This choice of potential allows us to separate the carrier motion along three coordinate axes. The 3D envelope wave function $F(r)$ can therefore be presented as a product of three 1D eigenfunctions ϕ_ξ in the following way:

$$F(r) = F_{n_x,n_y,n_z}(x,y,z) = \phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z) \qquad (5)$$

The 3D Schrödinger equation also decouples in this case into three identical one-dimensional (1D) quantum-well superlattices.

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial x}\frac{1}{m^*(x)}\frac{\partial}{\partial x} + V_x(x)\right]\phi_{n_x}(x) = E_{n_x}\phi_{n_x}(x) \qquad (6a)$$

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial y}\frac{1}{m^*(y)}\frac{\partial}{\partial y} + V_y(y)\right]\phi_{n_y}(y) = E_{n_y}\phi_{n_y}(y) \qquad (6b)$$

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z} + V_z(z)\right]\phi_{n_z}(z) = E_{n_z}\phi_{n_z}(z) \qquad (6c)$$

Here n_ξ denote the quantum number. The total energy spectrum for the wave function $F(r)$ is given by:

$$E_{n_x,n_y,n_z} = E_{n_x} + E_{n_y} + E_{n_z} \qquad (7)$$

Where E_n are the eigenvalues of the one-dimensional Schrödinger's equation.

For the chosen geometry of QDC and band offsets the carrier wave functions and energy spectrum are mostly determined by the nearest-neighbor interaction between dots separated by the potential barrier V_0.

The corner potentials induce only minor corrections, which are particularly small for the below-the-barrier states. This observation is important because the confining potential of Esq. (2) and (3) does not describe a simple QDC of a rectangular quantum dot surrounded by the potential barrier of the equal height.

In two dimensions, this situation is clear. Fig (2a) illustrates the two-dimensional confinement potential; with this configuration it is not possible to write the two-dimensional potential as a sum of two independent one-dimensional potential, and thus it is not possible to separate the x- and y-motions.

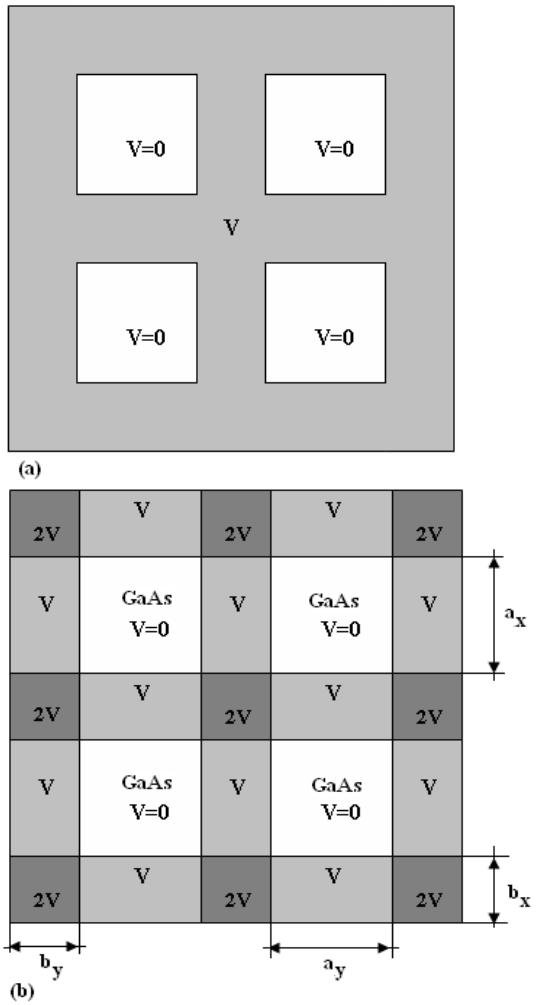

FIG.2. (a) the rectangular cross-section confinement potential ; and (b) an approximation form for the potential, suitable for decoupling the motion Note that the carrier states in quantum dots are mostly determined by interaction with nearest-neighboring dots separated from each other by the potential V0

However, a very loose approximation may be to write the potential as in Fig (2b) [8]. With this form, the potential does equal the sum of tow independent finite well potential. The approximation occurs in the corner region outside of the quantum dots where the two quantum well potential barrier heights V_0 sum to give $2V_0$. Similarly, in 3D, there exist outer regions where the overlap of 1D potentials along each axes gives rise to a potential barrier of $3V_0$.

The solution of Eq (1) with the potential of Eqs (2) and (3) has the form familiar from the Kronig–Penny model [9]. By using the transfer matrix method [10] and the boundary condition of Bastard [11], we arrive:

For $E_\xi > V_0$ (8a)

$$\cos(q_\xi d_\xi) = \cos(k_\xi^w a_\xi)\cos(k_\xi^b b_\xi) - \frac{1}{2}\left(R + \frac{1}{R}\right) \times \sin(k_\xi^w a_\xi)\sin(k_\xi^b b_\xi)$$

For $0 < E_\xi < V_0$ (8b)

$$\cos(q_\xi d_\xi) = \cos(k_\xi^w a_\xi)\cosh(k_\xi^b b_\xi) - \frac{1}{2}\left(-R + \frac{1}{R}\right) \times \sin(k_\xi^w a_\xi)\sinh(k_\xi^b b_\xi)$$

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$$R = \frac{k_\xi^B m_w^*}{k_\xi^w m_B^*} \quad (9)$$

where

$$k_\xi^w = \frac{1}{\hbar}\sqrt{2m_w^* E_\xi}\ , \quad k_\xi^b = \frac{1}{\hbar}\sqrt{2m_b^* \left|E_\xi - V_0\right|} \quad (10)$$

The effective masses m_w^* and m_b^* used in Eqs. (8). and (10) depend on the crystallographic orientation of the quantum dot interfaces. Equations (8) and (10) allow us to calculate the carrier dispersion relation in the QDC:

$$E(q) = E_x(q_x) + E_y(q_y) + E_z(q_z) \quad (11)$$

Since for each given value of q_ξ there is an infinite number of solutions, we use the miniband index n_ξ to label the carrier energy.

3. Numerical results

In this section, we show that despite the simplicity of the theoretical formalism used, it is capable of capturing new features characteristic for 3D artificial QDC that are not present in real bulk crystals and quantum well superlattices.

We carry out our analysis of the 3D minibands in the artificial QDC, on the example of GaAs/AlAs material system. In our calculations, we used the following values for the effective masses:

$$m_w^* = m_{GaAs}^* = 0.067 m_0\ ,\ m_b^* = m_{AlAs}^* = 0.15 m_0$$

We show in Fig.3 the electron dispersion in a simple cubic QDC along [100] crystallographic direction. The energy band structure following from Eqs (8), it is not surprising. In fact, it is expected from the format similarity between them and the Kroing-Penny relation of the superlattices. The carrier wave vector is denoted by q with subscript showing particular quasi crystallographic direction. Zero energy along the ordinate axis corresponds to the position of the potential barrier.

The results in Fig. 2 are shown for a QDC that consists of quantum dots with the size $a = 6.5nm$ and interdot distance $b = 1.5nm$. The energy bands are denoted by three quantum numbers $n_x n_y n_z$ with the superscript indicating the degeneracy of the band.

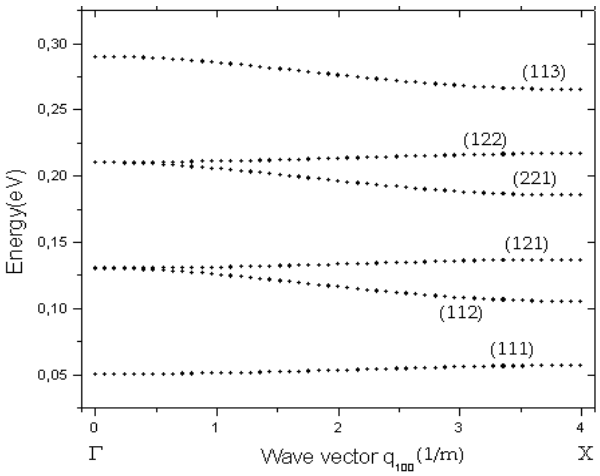

FIG. 3 Dispersion relation in a cubical QDC shown along [100] quasi crystallographic direction

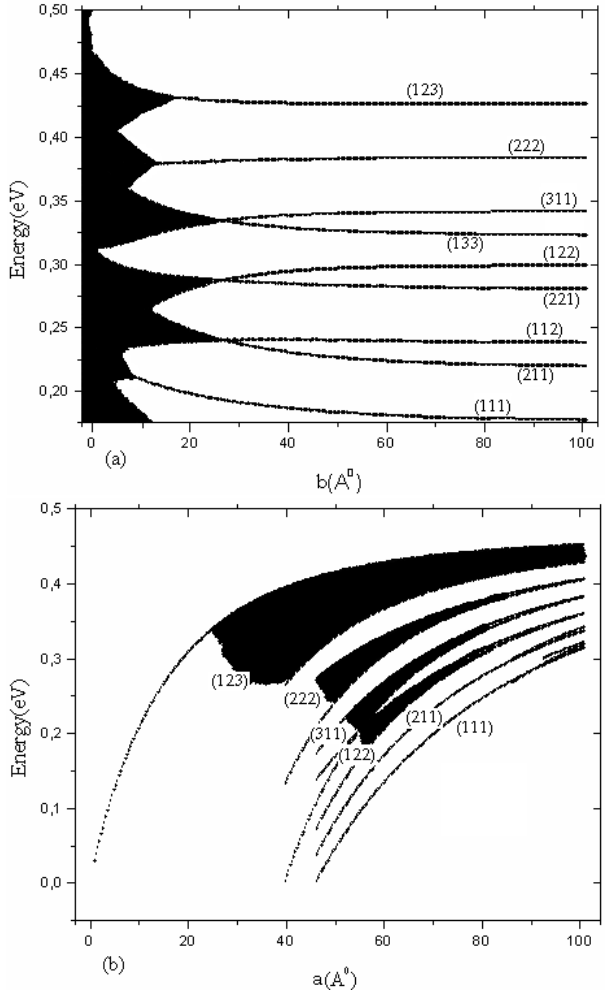

FIG. 4. (a) Miniband width as a function of the interdot distance. The size of the dots is 6.5nm. (b) Miniband energy as a function of dot size. The interdot distanc is 1.5nm.

The energy bands shown in Fig.3 are degenerated in the center of the quasi Brillouin zone (QBZ) of the artificial crystal. The highest, sixfold, degeneracy is achieved in minibands of cubical QDC characterized by different quantum numbers. If two of these three quantum numbers are equal, the degeneracy is threefold. Finally, if three quantum number are equal, there is no symmetry degeneracy in such a miniband. Moving from the point of high symmetry in the center of the QBZ to a point of lower symmetry, the energy bands split. This degeneracy is a result of the same symmetry of the dots and the superlattice. If their symmetries are different, the twofold degeneracy will be the maximum permitted in all directions.

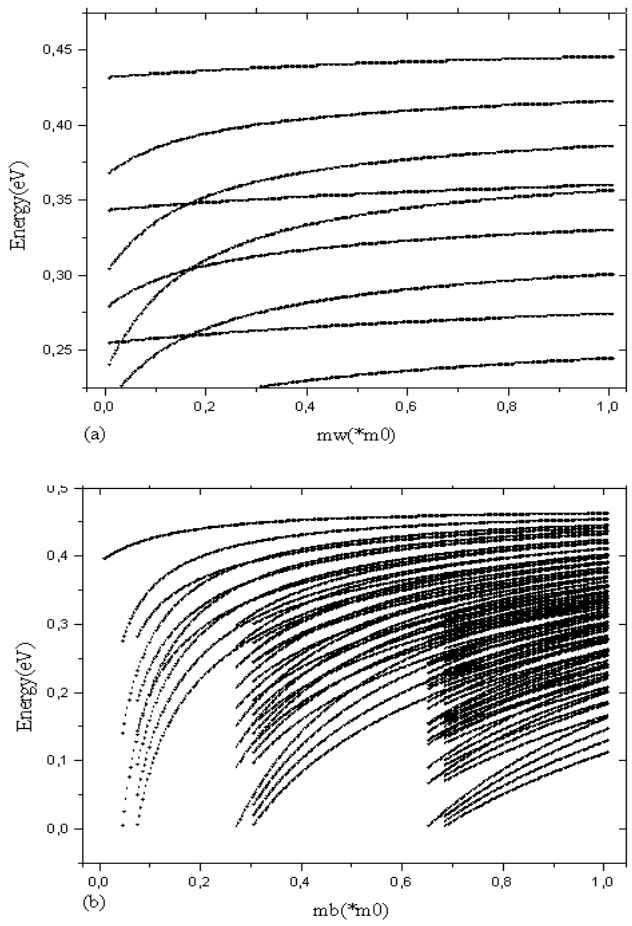

FIG.5. (a) Energy as a function of the masse in the well. (b) Energy as a function of the masse in the barrier

The formation of 3D minibands in QDC is illustrated in Figs. (4a) and (4b). It is well known that a single quantum dot has discrete spectrum below a potential barrier and continuous spectrum above the potential barrier. When quantum dots are separated by a finite barrier and positioned very close to each other so that there is a significant wave function overlap, the discrete energy levels split into minibands. This can be seen in Fig. (4a) for the interdot distance b below 3 nm. As the interdot distance increases, and the wave function overlap decreases, the minibands below the potential barrier reduce to discrete levels. This behavior is expected and consistent with what one observes in conventional quantum well superlattices. The 3D regimentation of quantum dots in QDC leads to appearance of "resonant" quasidiscrete energy levels above the potential barrier V_0 for large interdot distances (5 nm for GaAs/AlAs) as seen in Fig. (4a). Figure (4b) demonstrates a transformation of QDC minibands into discrete levels below the potential barrier and quasicontinuum above the barrier. Other important observations to make in Fig. (4b) are that the miniband width does not increase monotonously with the energy, and that for realistic interdot distances complete energy gaps (stop bands) are formed in QDC.

We can have the same information about the formation the minibands structure in GaAs/AlAs-QDC by the variation of the barrier and well masses (see Fig.5.)

4. Conclusion

Quantum dot superlattices QDSLs offer prospects for new generation of semiconductor devices. In particular; the GaAs/AlAs-QDSLs have attracted considerable attention due to application for infrared photodetector.

In this paper, the carrier band structure in a 3D *regimented* array of semiconductor quantum dots QDC has been analyzed. Numerical simulations have been carried out for the conduction band of a GaAs/AlAs quantum dot crystals. It was shown that the coupling among quantum dots leads to a splitting of the quantized electron energy levels of single dots, which results in the formation of 3D minibands. By changing the size of quantum dots, interdot distances, barrier height, and regimentation, one can control the electronic band structure of this artificial crystal. The properties of the artificial crystals turned out to be more sensitive to the dot regimentation than to the dot shape.

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