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Influence of quantum dot shape on energy spectra of three-dimensional quantum dots superlattices

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The superlattices of quantum dots *InAs* in a matrix *GaAs* has been studied in this work. The superlattices of spherical and cubic quantum dots (QD) has been studied. Using the method of plane waves for different shapes of QD, analytical expressions for calculating the energy spectrum has been obtained. The dependences of energy zones at high symmetry dots has been constructed. Dependences of widths of zones has been found. It effects on the optical properties and, accordingly, the absorption and radiation coefficients. It has been shown that the largest bandwidth is for QD with the smallest symmetry (cubic quantum dots).

Keywords: superlattice, quantum dot, form of quantum dot, electron spectrum, zone width.

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Introduction

Quantum dot (QD) lasers based on the $A_{III}B_V$ compound, one of the large modern practical applications of quantum dots [1-3]. Theoretically, the expected benefits of such lasers (low limit current (about 10 A/cm^2)), high gain, temperature stability of the limit current) have been tested. For telecommunications, the most desirable in practice is the range of maximum transparency of the fiber - wavelength $1.3 - 1.5 \mu\text{m}$. It is at a wavelength of $1.3 \mu\text{m}$ (that is, the maximum transparency of the optical fiber) that lasers are emitted and realized at quantum dots *InAs* in the matrix *GaAs* [4-5].

For further improvement of optoelectronic devices, it is necessary to conduct both experimental and theoretical studies of the physical properties of the structures of spatially ordered quantum dots. Therefore, the superlattice of quantum dots has attracted a lot of attention in recent years [6-10]. The authors of work [11] considered the superlattices of the cubic quantum dots *GaAs/AlAs*, which are widely used in infrared photodetectors. Using the approximation of the envelope function in the Kronig-Penney model, the authors showed that taking into account the overlap integrals

with decreasing distances between QDs leads to the formation of three-dimensional minizones. However, the authors limited themselves to considering the energy spectrum of these electronic 3D-subbands, stating that it is more sensitive to the parameters of the superlattice of cubic quantum dots (SCQD) than to the shape of the QDs themselves. In work [12], the method of joined flat waves consists in calculating the electronic zone structure in the supergrate of spherical quantum dots (SSQD) in the approximation of effective masses. The influence of QDs size and the distance between them on the position of the energy bands and their width had investigated.

Studies have shown that the form of the QD significantly affects the energy spectrum of quasiparticles [13]. Experimental work shows a difference from spherical [14-16], which ultimately affects the optical properties of materials. However, most of the work is devoted to spherically symmetric QDs due to its simpler solution. Linear and nonlinear absorption coefficients at QDs of spherical shape had calculated in [17]. Attention was drawn to the ellipsoidal shape in relation to the more realistic comparison with the experimental size of QDs [15].

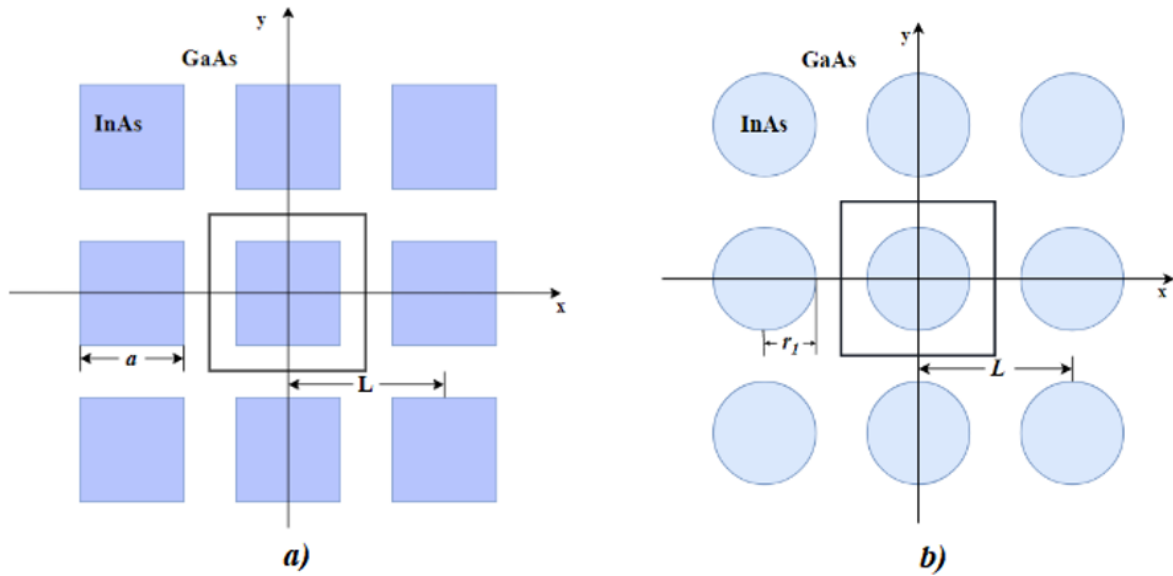


Fig.1. Parameters of superlattices for a) cubic QDs; b) spherical QDs.

The blurring of the spectrum due to the heterogeneity of the shapes and sizes of QDs requires experimenters to create a uniform array of QDs. The high density of quantum dots can also lead to the formation of high-width energy zones, which will increase the temperature dependence of laser radiation characteristics.

Therefore, it had the ordered arrays of quantum dots with small variance in size and shape that are important from the point of view of applied value. The aim of this work is to calculate the width of the electronic zone structure of an ordered array of spherical QDs using an example of a three-dimensional superlattice of nanocrystals *InAs* arranged in a *GaAs* medium of different shapes (spherical, cubic). In most cases, the shape of quantum dots grown in superlattices is uncertain. So our task is to study the effect of shape on the electron spectrum by the method of plane waves.

I. Electron energies of semiconductor quantum dots

Let us to consider the SSQD and SCQD *InAs*, placed in a matrix *GaAs* (Figure 1). Three-dimensional superlattices of quantum dots (cubic, spherical), which are located in the nodes of a cubic superlattice, the elementary cell of which is in the form of a cube, are investigated. We introduce the following notation: r_1 – radius of a spherical quantum dots (QD) in SSQD; a – the length of the edge of the QD; L – distance between centers of QD.

To find the energy spectrum and wave functions of an electron, we solve the electron Schrödinger equation:

$$H_e \psi_e(r_e) = E \psi_e(r_e), \quad (1)$$

with electron Hamiltonian:

$$H_e = \mathbf{P} \frac{1}{2m_e^*(x, y, z)} \mathbf{P} + V_e(x, y, z), \quad (2)$$

where:

$$V_e(x, y, z) = \begin{cases} 0, & x^2 + y^2 + z^2 \leq r_1^2 \\ V_{0e}, & \text{others} \end{cases},$$

$$m_e^* = \begin{cases} m_1, & x^2 + y^2 + z^2 \leq r_1^2 \\ m_2, & \text{others} \end{cases},$$

for SSQD and

$$V_e(x, y, z) = \begin{cases} 0, & |x| \leq \frac{a}{2}, |y| \leq \frac{a}{2}, |z| \leq \frac{a}{2} \\ V_{0e}, & \text{others}, \end{cases}$$

$$m_e^* = \begin{cases} m_1, & |x| \leq \frac{a}{2}, |y| \leq \frac{a}{2}, |z| \leq \frac{a}{2} \\ m_2, & \text{others} \end{cases}$$

for SCQD. m_1 and m_2 – effective electron masses in *InAs* and *GaAs*, accordingly.

The wave function of the electron $\psi_e(r_e)$ must gratify the periodicity condition. Let's write it in the form:

$$\psi_e(r_e) = \frac{1}{(\sqrt{L})^3} \sum_{n_x, n_y, n_z} c_{n_x, n_y, n_z} e^{i(k_{n_x}x + k_{n_y}y + k_{n_z}z)}, \quad (3)$$

where

$$k_{n_x} = k_x + n_x K, \quad k_{n_y} = k_y + n_y K, \quad k_{n_z} = k_z + n_z K, \quad (4)$$

$$K = \frac{2\pi}{L}, \quad \mathbf{k}(k_x, k_y, k_z), \quad n_x, n_y, n_z = 0, \pm 1, \pm 2, \dots$$

When we put (2) and (3) in (1), multiplying from the

left by $\frac{1}{(\sqrt{L})^3} e^{-i(k'_{nx}x+k'_{ny}y+k'_{nz}z)}$ and integrate throughout the region, the matrix elements of Hamiltonian (1) for

spherical QDs had gotten in the form of:

$$-h^2 c_{n_x, n_y, n_z} \left[\left(\frac{1}{2m_2} \delta_{n_x n'_x} \delta_{n_y n'_y} \delta_{n_z n'_z} + \frac{1}{2m_2 L^3} Q \right) \times (k_{nx} k'_{nx} + k_{ny} k'_{ny} + k_{nz} k'_{nz}) + \left(\delta_{n_x n'_x} \delta_{n_y n'_y} \delta_{n_z n'_z} - \frac{Q}{L^3} \right) \times V_{0e} \right], \quad (5)$$

for cubic QDs:

$$-h^2 c_{n_x, n_y, n_z} \left[\left(\frac{1}{2m_2} \delta_{n_x n'_x} \delta_{n_y n'_y} \delta_{n_z n'_z} + \frac{1}{2m_2 L^3} D_i D_j D_k \right) \times (k_{nx} k'_{nx} + k_{ny} k'_{ny} + k_{nz} k'_{nz}) + \left(\delta_{n_x n'_x} \delta_{n_y n'_y} \delta_{n_z n'_z} - \frac{D_i D_j D_k}{L^3} \right) \times V_{0e} \right], \quad (6)$$

where:

$$\begin{aligned} \frac{1}{2m_2} &= \frac{1}{2m_1} - \frac{1}{2m_2}, \quad k'_{nx} = k_x + n'_x K, \quad k'_{ny} = k_y + n'_y K, \quad k'_{nz} = k_z + n'_z K, \\ Q &= \begin{cases} \frac{4}{3} \pi r_1^3, & n_x = n'_x, n_y = n'_y, n_z = n'_z, \\ \frac{4\pi(-r_1 K \lambda \cos(r_1 K \lambda) + \sin(r_1 K \lambda))}{(K \lambda)^3}, & n_x \neq n'_x, a\delta o n_y \neq n'_y, a\delta o n_z \neq n'_z, \end{cases} \quad (7) \\ \lambda &= \sqrt{(n_x - n'_x)^2 + (n_y - n'_y)^2 + (n_z - n'_z)^2}, \quad s = (i, j, k) \\ D_s &= \begin{cases} \frac{a}{L}, & n_x = n'_x, n_y = n'_y, n_z = n'_z, \\ \frac{\sin(\pi(n_s - n'_s) \frac{a}{L})}{\pi(n_s - n'_s)}, & n_x \neq n'_x, a\delta o n_y \neq n'_y, a\delta o n_z \neq n'_z, \end{cases} \\ \delta_{n_q, n'_q} &= \frac{1}{L} \sum_{n_q, n'_q} \int_{-\frac{L}{2}}^{\frac{L}{2}} e^{i(k_{nq} - k'_{nq})q} dq, \quad q = (x, y, z). \end{aligned}$$

Therefore, we can calculate the electron structures for given structures.

Results

Specific calculations had performed for heterosystem *InAs/GaAs* with the following parameters: $m_1 = 0.067$, $m_2 = 0.023$, $V_{0e} = 0.77eV$. In this paper we had used such a number of plane waves n_x, n_y, n_z that provided accuracy in calculations with an error of 0.1 %.

To compare the effect of the shape of the QDs on the energy spectrum, the following two approximations were made: first, QDs have the same volumes, so the sizes are proportional; second, in all types of superlattices, the elementary cell is the same as the cube. The second approximation is equivalent to the fact that superlattices have the same density of QDs. To ensure the same volume based on a spherical QD with radius r_1 . Figure 2 schematically shows QDs of different forms with the same volume.

Depending on the spherical QDs, the following parameters had selected for the cubic QDs:

$$a = r_1 \cdot 3 \sqrt[3]{\frac{4}{3} \pi},$$

Consider the electron energy spectrum in the cubic lattice of QDs (Fig. 3) with $k_z = 0$. The figure shows that the qualitative dependence of the energy spectrum is the same.

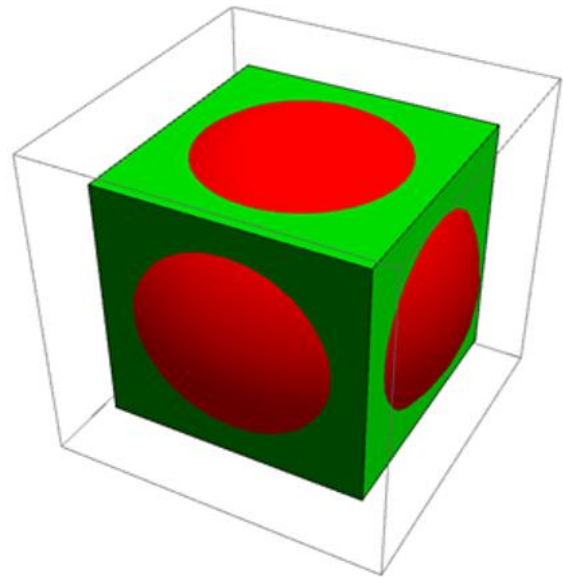


Fig. 2. Schematic representation of QDs of different forms of the same volume.

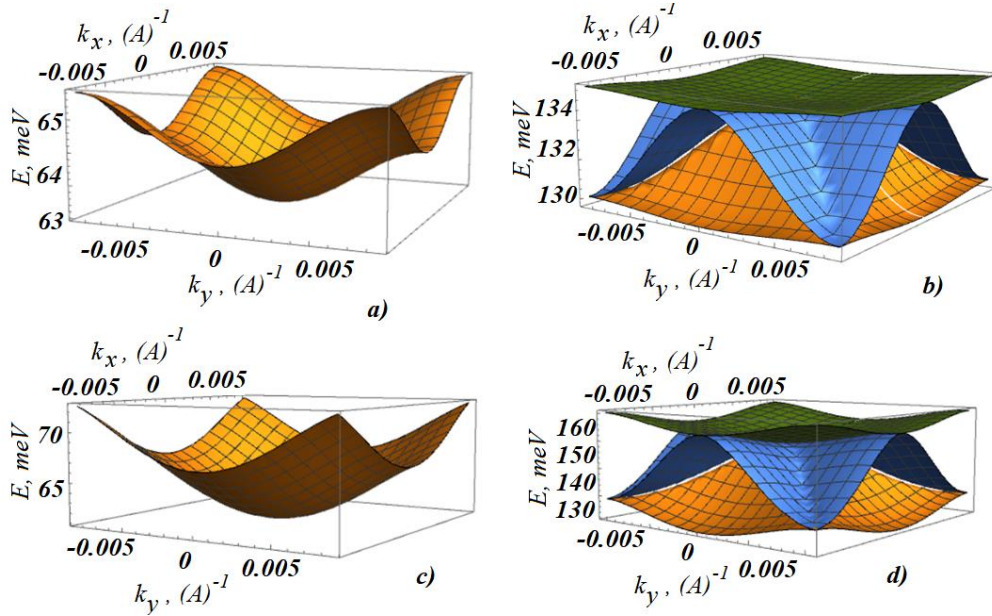


Fig. 3. The energy dependence of the first minizone of electron for a) SCQD; c) SSQD on the two-dimensional wave vector $\vec{k}(k_x, k_y, k_z = 0)$. The energy dependence of the following minizones for b) SCQD; d) SSQD on the

two-dimensional wave vector $\vec{k}(k_x, k_y, k_z = 0)$, де $a = r_1 \sqrt[3]{\frac{4\pi}{3}}$, $L = 192 \text{ \AA}$, $r_1 = 90 \text{ \AA}$.

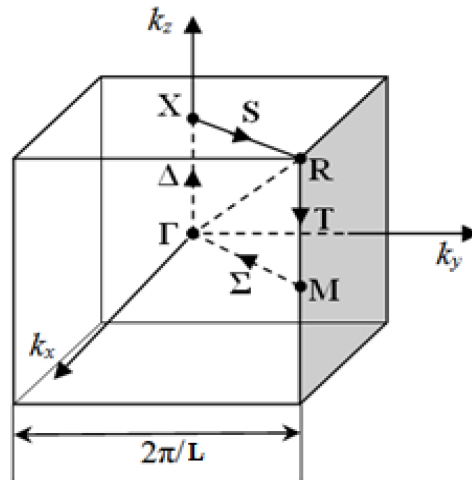


Fig. 4. Brillouin zone of a three-dimensional superlattice of QDs.

For the convenience of energy spectrum analysis, we had used high symmetry dots of the k-space of the superlattice of quantum dots of cubic symmetry. It had shown on Figure 4. The high symmetry dots are as follows:

$$\Gamma(0,0,0), \quad X\left(0,0,\frac{\pi}{L}\right), \quad M\left(\frac{\pi}{L},\frac{\pi}{L},0\right),$$

$$R\left(\frac{\pi}{L},\frac{\pi}{L},\frac{\pi}{L}\right), \quad \text{and characteristic directions} \quad -$$

$$\Delta\{\Gamma \rightarrow X\}, \quad S\{X \rightarrow R\}, \quad T\{R \rightarrow M\},$$

$$\Sigma\{M \rightarrow \Gamma\}.$$

Figure 5 shows the electron spectra of four minizones for QDs of different shapes, calculated according to formulas (5) to (7) for the radius of the sphere.

The nature of the dependence of the energy spectrum is the same. The figure shows that the maximum energy of the first minizone had reached at R, the minimum - at Γ . If we consider the II, III and IV minizones, then the maximum energy at M, the minimum at X. The graphs also show that zones II, III and IV are three times degenerate at G and R.

We have compared the widths of the zones of QD arrays formed by QD of different shapes (Figure 6). The graphs show that as the radius R increases (i.e., as the volume of QD increases), the energy of all states decreases, regardless of the shape of the QD. This is due to the fact that the energy of the electron in the isolated QD decreases, the probability of the electron in the QD increases. Accordingly, the probability of tunneling the

electron into other QDs decreases. In addition, it can be seen that the cubic QD has a wider zones width compared to the spherical QD. This is due to the fact that in cubic QD the electron has greater limitations in motion than in spherical QD.

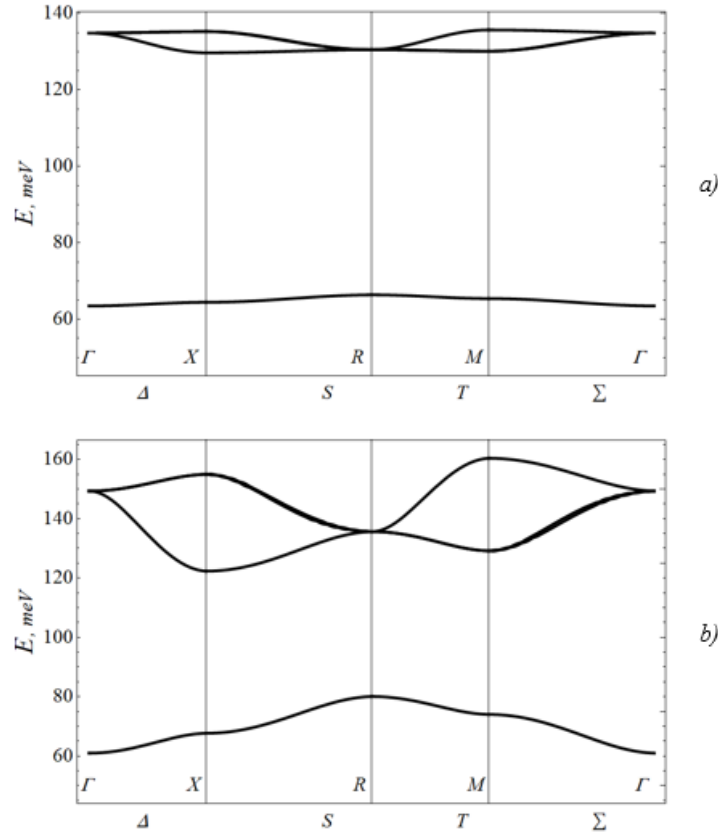


Fig. 5. Electron energy spectra of the first and subsequent excited minizones of the superlattice of QDs for a) spherical QDs; b) cubic QDs, where $a = r_1 \sqrt[3]{\frac{4\pi}{3}}$, $L = 192 \text{ \AA}$, $r_1 = 90 \text{ \AA}$.

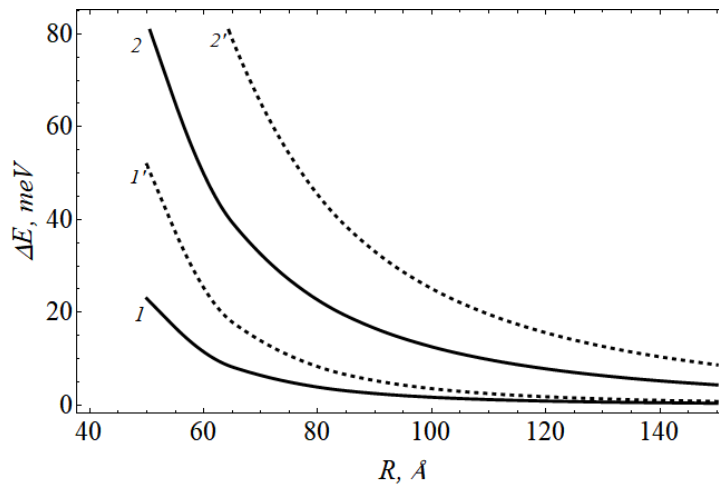


Fig. 6. Lattice width dependence on radius of spherical and cubic QDs. Solid line denotes the width of the first zone of the lattice (1, 2) and a dotted line - the second zone (1', 2'). 1,1'- zone widths for SSQD; 2,2'- zone widths for SCQD.

Conclusion

In the paper had considered the three-dimensional superlattice of QDs InAs placed in the matrix GaAs. QDs had chosen of different forms: spheres, cubes, with the same volumes. Using the theory of plane waves, the energies of the ground and first excited states had calculated. Using high symmetry dots in the Brillouin zone, the energy spectrum of the electron had calculated. And also the dependence of the widths of the zones of quantum dots of different forms had calculated, which will most likely affect the optical properties, namely the absorption and radiation coefficients. The proposed

method of calculating the band spectra of QD superlattices can also be applied to cylindrical [18] QDs, hole states [19] taking into account heteroboundary stresses and polarization effects [20].

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Вплив форми квантової точки на енергетичні спектри тримірних надграток квантових точок

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Визначено зонний спектр надграток квантових точок різної форми у точках високої симетрії. Розглянуто кубічні, циліндричні та сферичні квантові точки. Обчислено ширини мінізон. Встановлено залежності мінізон від геометричних розмірів квантових точок та їх концентрації.

Ключові слова: надрешітка, квантова точка, форма квантової точки, електронний спектр, ширина зони.