PHYSICS AND CHEMISTRY OF SOLIDSTATE
V. 18, № 2 (2017) P. 151-157
DOI: 10.15330/pcss.18.2.151-157

ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 18, № 2 (2017) С. 151-157

PACS: 68.65.Cd, 78.67.Pt

ISSN 1729-4428

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Coefficient of Interband Light Absorption by $InAs/Ga_xIn_{1-x}As$ Quantum Dot Superlattice at Low Temperatures

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In the paper the $InAs/Ga_xIn_{1-x}As$ superlattice system of small size cubic QDs (10 nm) has been considered. Dispersion relations for electron and hole subbands have been calculated for superlattices of different dimensionality. The dependences of the interband absorption coefficient on light frequency, quantum dot size and interdot distance have been researched.It is shown, that the dimension of the superlattice has influence on the shape of the absorption bands and the increasing of the distance between quantum dots is followed by narrowing of the absorption peaks for all three superlattice types.

Key words: quantum dot, superlattice, electronic states, absorption coefficient.

Article acted received 07.04.2017; accepted for publication 05.06.2017.

Introduction

Superlattices on the base of 2D quantum wells are quite well researched and widely used in optoelectronics devices [1, 2]. In particular, lasers based on InGaAs/GaAs quantum wells are broadly utilized for fiber connection. Significantly high threshold currents, low operating temperature and low temperature stability of these lasers do not always meet the requirements needed for high-speed communication devices. Progress in making multilayer structures of self-assembled quantum dot III-V compounds, which are quite uniform in size and shape and are characterized by large surface density, led to the creation of semiconductor lasers based on quantum dots. These lasers can generate radiation with an actual wavelength of $\lambda = 1.3$ mkm with extremely low threshold currents and high power output. Optical amplifiers based on quantum-dot structures are extremely important for high-speed signal processing. They allow the processing of signals at speeds of over 40 Gbit/s.

To further improve optoelectronic devices, it is necessary to carry out both experimental and theoretical studies of physical properties of spatially assembled quantum dot (QD) structures. Therefore, quantum dot superlattices attract great attention of researchers in the last years. The authors of [3] examined GaAs/AlAs cubic quantum dot superlattices (CQDS), which are widely used in infrared photo detectors. Using the envelope function approximation in the Kronig-Penney model, the authors showed that taking into account overlapping integrals with decreasing interdot distances results in the appearance of three-dimensional minibands. However, the authors confined their attention to the energy spectrum of these electronic 3D subbands, noting that it is more sensitive to the parameters of a CQDS than a quantum dot shape.

In Reference [4] in the effective mass approximation the electronic band structure in a spherical quantum dot superlattice (SQDS) was calculated by augmented plane wave method. The effect of QD size and interdot distance on the position of the energy bands and their width was investigated.

Theoretical study of electronic band structure of the GaAs/AlAs superlattice with uniformly distributed tunnel-connected QDs was done in [5, 6]. The relations of wave vector dependence of the electron energy were obtained. Optical properties of the CQDS were also studied. Specifically, the matrix element and electronic density of states of intersubband transitions from the ground state to the first excited states of the superlattice were calculated at different QD radii and interdot distances. The resulting calculation made it possible to investigate the dependence of intersubband absorption coefficient of the $GaAs/Al_xGa_{1-x}As$ heterosystems with periodically assembled spherical quantum dots on the frequency of the incident light.

The investigation of optical properties of non-interacting quantum dots systems [7, 8] showed that the average size of quantum dots is the critical parameter. Along with it their shape is also important. It is obvious that for tunnel-coupled quantum dot systems the QD size,

shape and interdot distance are important parameters. In the present paper the InAs/$Ga_xIn_{1-x}As$ superlattice system of small size cubic QDs (10 nm) has been considered. Dispersion relations for electron and hole subbands have been calculated for superlattices of different dimensionality. The dependences of the interband absorption coefficient on light frequency, quantum dot size and interdot distance have been researched.

I. Setting of the problem

The study of absorption spectra is one of the important methods to determine physical characteristics of quantum dot heterosystems. To determine them we consider the system of spatially assembled cubic quantum dots of equal size that are embedded in the matrix, as it is shown in Figure 1, i.e., a cubic quantum dot superlattice.

If $a_1 = a_2 = a_3$, a CQDS will be referred to as a 3D-superlattice, when $a_3 = a_1 \quad a_2$, 2D-superlattice, and for $a_3 \quad a_1 = a_2$, 1D-superlattice. It is clear that the translation vector of the superlattice is

$$\vec{n} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3,$$

where n_i $(0, \pm1, \pm2, ...)$, $\vec{a}_i$ $(i = 1, 2, 3)$ are basic translation vectors, their directions coincide with the axes of the Cartesian coordinate system.

The theoretical research of the nanoheterosystem of wide-gap semiconductors involves solving the Schrödinger equation for an electron. The problem can be solved by various methods: the finite elements [10], augmented plane waves [11], or pseudopotential [12]. We consider the CQDS with small size (2-10 nm) semiconductor quantum dots, which are characterized by size quantization of charged particles. In view of this, we employ the parabolic band approximation and the effective mass approach to determine the energies and wave functions of not only electrons but also holes (heavy holes).

The Schrödinger equation which describes the motion of a charged particle (electron or hole) in the CQDS can be written as follows:

$$\left[-\frac{\mathbf{h}^2}{2}\nabla\frac{1}{m(\vec{r})}\nabla + V(\vec{r})\right]\psi_\nu(\vec{r}) = E\psi_\nu(\vec{r}), \qquad (1)$$

where $V(\vec{r}) = \begin{cases} 0, & \begin{cases} n_1a_1 \le x \le n_1a_1 + L \\ n_2a_2 \le y \le n_2a_2 + L \\ n_3a_3 \le z \le n_3a_3 + L \end{cases} \\ U_0, & \text{in another region of space,} \end{cases}$ is the periodic potential $V(\vec{r})$, which corresponds to an infinite sequence of cubic quantum dots, $m(\vec{r})$ is the effective mass of a particle.

Using the approximation to find the particle potential energy, we write the potential $V(\vec{r})$ in the form of a sum of three independent periodical coordinate functions *x*, *y* and *z*:

$$V(\vec{r}) = V(x) + V(y) + V(z), \qquad (2)$$

This choice of the potential allows one to split the motion of a charged particle in three directions. Three-dimensional Schrödinger equation (1) in this case will be written in the form of three identical one-dimensional equations. Then the envelope wave function of equation (1) can be represented as a product of three one-dimensional eigenfunctions

$$\psi_\nu(\vec{r}) = \psi_{\nu_1,\nu_2,\nu_3}(x_1, x_2, x_3) = \varphi_{\nu_1}(x_1)\cdot\varphi_{\nu_2}(x_2)\cdot\varphi_{\nu_3}(x_3), \quad (3)$$

and the energy as a sum of three corresponding components

$$E_\nu = E_{\nu_1} + E_{\nu_2} + E_{\nu_3}. \qquad (4)$$

It is necessary to use the following equation to determine E_{ν_i} and φ_{ν_i}:

$$\left[-\frac{\mathbf{h}^2}{2}\frac{\partial}{\partial x_i}\frac{1}{m(\vec{r})}\frac{\partial}{\partial x_i} + V(x_i)\right]\varphi_{\nu_i}(x_i) = E_{\nu_i}\varphi_{\nu_i}(x_i),$$
$$i = 1, 2, 3, \qquad (5)$$

Shrödinger equations (5) correspond to the well-known Kronig-Penney model. According to this model, the solution of equation (5) is known [12] and determined from the relevant dispersion relations in different regions of the superlattice [3].

If $0 < E_\nu < U_0$, the dispersion relation is written as

$$\cos(k_i a_{\nu_i}) - \cos(\chi_{\nu_i} L)\,\mathrm{ch}(\xi_{\nu_i} d) + \frac{\left(\chi_{\nu_i} m_2\right)^2 - \left(\xi_{\nu_i} m_1\right)^2}{2\chi_{\nu_i} m_2 \cdot \xi_{\nu_i} m_1}\sin(\chi_{\nu_i} L)\,\mathrm{sh}(\xi_{\nu_i} d) = 0, \qquad (6, a)$$

when $E_\nu > U_0$,

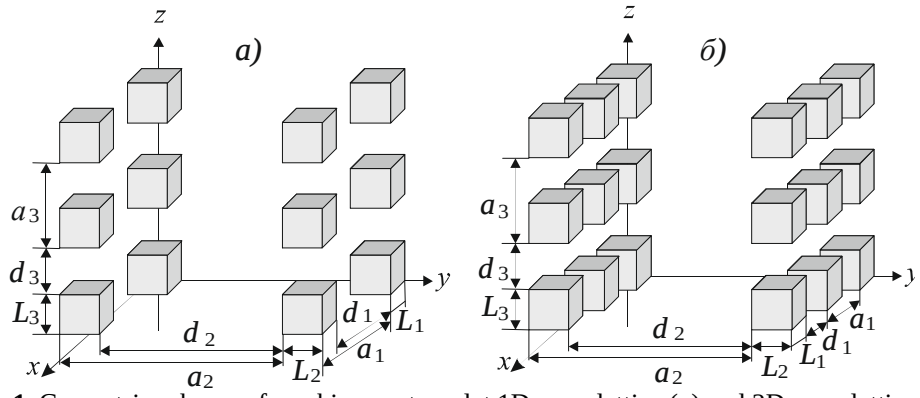

Fig. 1. Geometric scheme of a cubic quantum dot 1D-superlattice (*a*) and 2D-superlattice (*b*).

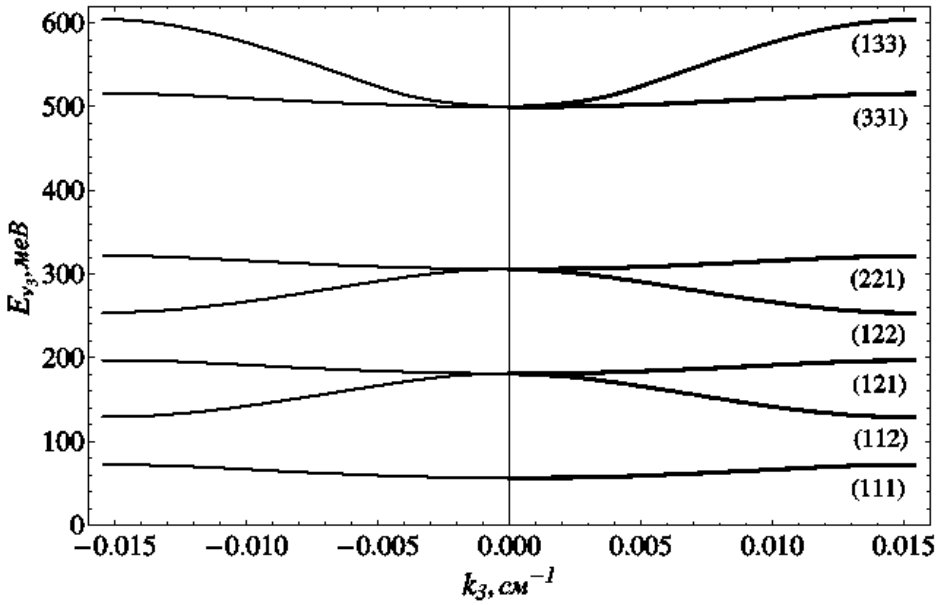

Fig. 2. Energies of electron states in the CQDS $L = 96\,\text{Å}, d = 12\,\text{Å}$.

$$\cos(k_i a_{\nu_i}) - \cos(\chi_{\nu_i} L)\cos(\xi_{\nu_i} d_{\nu_i}) + \frac{\left(\chi_{\nu_i} m_2\right)^2 + \left(\xi_{\nu_i} m_1\right)^2}{2\chi_{\nu_i} m_2 \cdot \xi_{\nu_i} m_1}\sin(\chi_{\nu_i} L)\sin(\xi_{\nu_i} d_{\nu_i}) = 0, \quad (6, б)$$

where $\chi_{\nu_i} = \sqrt{\frac{2m_1\left(U_0 + E_{\nu_i}\right)}{\mathbf{h}^2}}$, $\xi_{\nu_i} = \sqrt{\frac{2m_2\left|E_{\nu_i}\right|}{\mathbf{h}^2}}$, m_1, m_2 are effective masses of a quasiparticle inside and outside the QD. Thus,

$$E_{\nu}(\mathbf{k}) = \sum_{i=1}^{3} E_{\nu_i}(k_i),\ \nu = \{\nu_1, \nu_2, \nu_3\}. \quad (7)$$

We assume that the monochromatic electromagnetic wave is incident on the quantum dot superlattice with the vector potential

$$\mathbf{A} = -\frac{ic}{\omega}\boldsymbol{\xi} A_0 e^{i(\boldsymbol{\chi}\mathbf{r} - \omega t)}, \quad (8)$$

where $\boldsymbol{\xi}, \boldsymbol{\chi}$ are polarization and wave vectors of the incident light respectively. The operator of the interaction of the electromagnetic wave (8) with an electron is expressed in the form

$$H' = \frac{e\mathbf{h}}{m_0\omega} e^{i(\boldsymbol{\chi}\mathbf{r} - \omega t)} A_0\left(\boldsymbol{\xi}, \nabla\right), \quad (9)$$

Here A_0 is the amplitude of the vector potential, ω is the frequency of the incident wave. Further we shall consider the case of linearly polarized light with the polarization vector directed along the Oz axis.

We consider the probability of electron transitions from the valence band with quantum numbers of the initial state $\lambda(v, \mathbf{k})$ to the final state $\lambda'(c, \mathbf{k}')$ (the conduction band), where v, v' are sets of quantum numbers of holes and electrons, respectively. The absorption coefficient which is determined by the difference of absorbed and emitted light is written [13]

$$\alpha = \frac{4\pi e\mathbf{h}}{Vm_0^2 cn\omega}\sum_{\lambda,\lambda'}\left|\boldsymbol{\xi} J_{\lambda\lambda'}\right|^2 \left(f(\lambda) - f(\lambda')\right)\delta\left[E_{\lambda'} - E_{\lambda} - \mathbf{h}\omega\right], \quad (10)$$

$f(\lambda) = \frac{1}{\exp\frac{E_\lambda - E_F}{k_0 T} + 1}$, $f(\lambda') = \frac{1}{\exp\frac{E_F - E_{\lambda'}}{k_0 T} + 1}$ are functions of distribution of charge carriers in the respective bands. In the dipole approach and the envelope function approximation the matrix element of a quantum transition is expressed by

$$J_{\lambda\lambda'} = \int \psi_{\lambda'}^* U_{\lambda'}^* \frac{\partial}{\partial z}\left(\psi_\lambda U_\lambda\right) dV, \quad (11)$$

U_λ is the Bloch oscillation function of the QD crystal at the point $k = 0$.

The absorption coefficient of the CQDS (10) at low (helium) temperatures under the condition of a complete occupation of the valence band and the free conduction band with electrons takes the form

$$\alpha = \frac{4\pi e\mathbf{h}K}{Nm_0^2 cn_0\omega}\sum_{\lambda\lambda'}\sum_{k}\left|I_{\lambda\lambda'}(\mathbf{k})\right|^2 \delta\left[E_{\lambda'}(\mathbf{k}) - E_\lambda(\mathbf{k}) - \mathbf{h}\omega\right], \quad (12)$$

where $I_{\lambda\lambda'}^2(\mathbf{k}) = \left|\int \psi_{\lambda'}^*(\mathbf{r})\psi_\lambda(\mathbf{r})dV\right|^2$ is a squared matrix element of the overlapping integral, $K = \left|\int_\Omega U_c^*(\mathbf{r})\frac{\partial}{\partial z}U_v(\mathbf{r})dV\right|^2$ is the Kane parameter.

II. Analysis of the results

The specific calculations have been performed for cubic quantum dot superlattices of the InAs/Ga_xIn_{1-x}As heterosystem with the following parameters:

$$m_{1e} = 0.023\, m_0,\ m_{2e} = (0.023 + 0.044x)\, m_0,$$
$$V_e = 0.77\ \text{åÂ}$$

$m_{1h} = 0.55\ m_0$, $m_{2h} = (0.55 + 0.04x)\, m_0$, $V_h = 0.33$ åÂ

For a cubic quantum dot 3D-superlattice we assume a quantum dot size to be $L = 96$ Å and equal interdot distances in different directions $d_x = d_y = d_z = d$. In case of a 2D-superlattice the following conditions should be satisfied: $d_3 = d_1 \quad d_2$, and for a 1D-superlattice: $d_3 \quad d_1 = d_2$.

Figure 3 presents the photon energy dependence of the absorption coefficient of the InAs/$In_{0.85}Ga_{0.15}As$ 3D-CQDS. Calculations were performed for quantum dots of different sizes L = 96 Å, 84 Å, 60 Å and the interdot distance d = 12 Å. It is seen from the graphic dependences that for L = 96 Å (curve 1) there are three absorption bands of different amplitudes and widths due to the presence of the corresponding number of electronic subbands at such sizes. While at L = 84 Å (curve 2) and L = 60 Å (curve 3) there are two and one absorption bands, respectively. A characteristic feature of the curves is the presence of peaks inside the absorption band similar to the 2D CQDS (Fig. 3). With decreasing the QD size there is an increase in the amplitude of the absorption coefficient, an expansion of bands and their shift towards higher frequencies of the incident light. A similar pattern is observed for the 1D CQDS (Fig. 4) but in contrast to the three-dimensional lattice there are the maximums of the absorption coefficient at the edges of

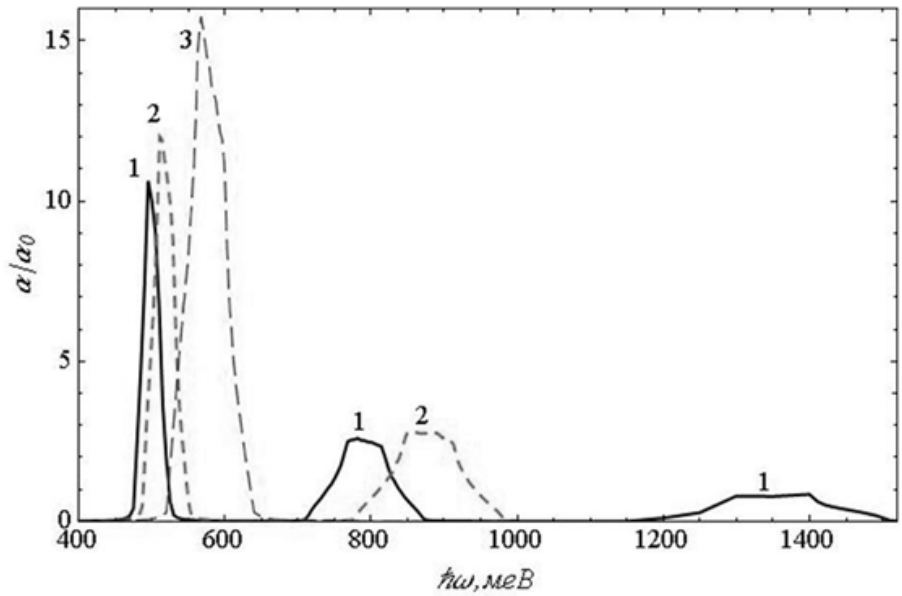

Fig. 3. Light absorption coefficient in InAs/$In_{0.85}Ga_{0.15}As$ 3D-CQDS at different quantum dot sizes: L = 96 Å (curve 1); L = 84 Å (curve 2); L = 60 Å (curve 3) and the interdot distance d=12 Å.

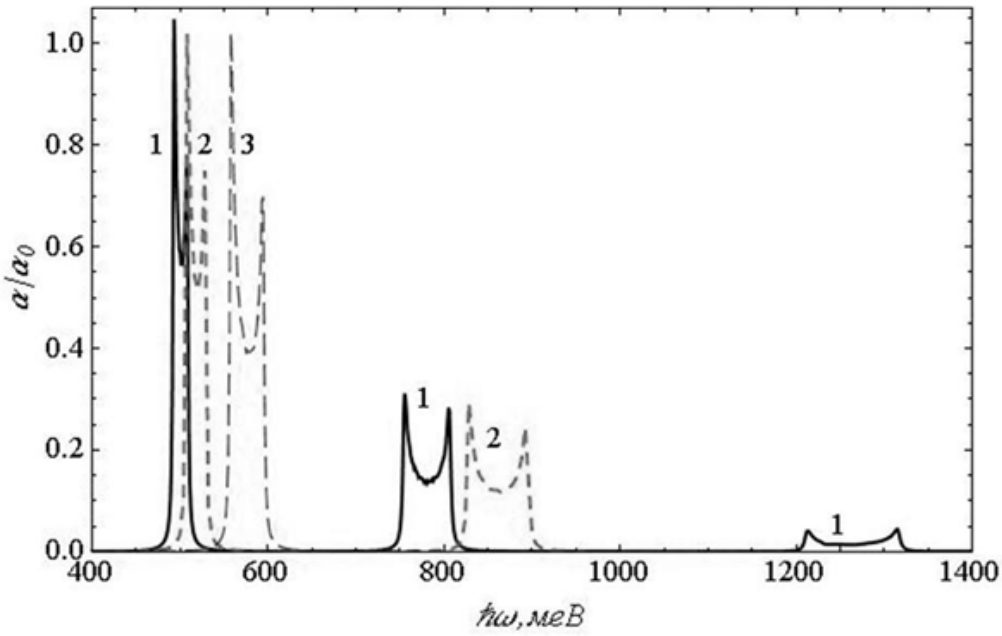

Fig. 4. Light absorption coefficient in InAs/$In_{0.85}Ga_{0.15}As$ 1D-CQDS at different quantum dot sizes: L=96 Å (curve 1); L=84 Å (curve 2); L=60 Å (curve 3) and the interdot distance d=12 Å.

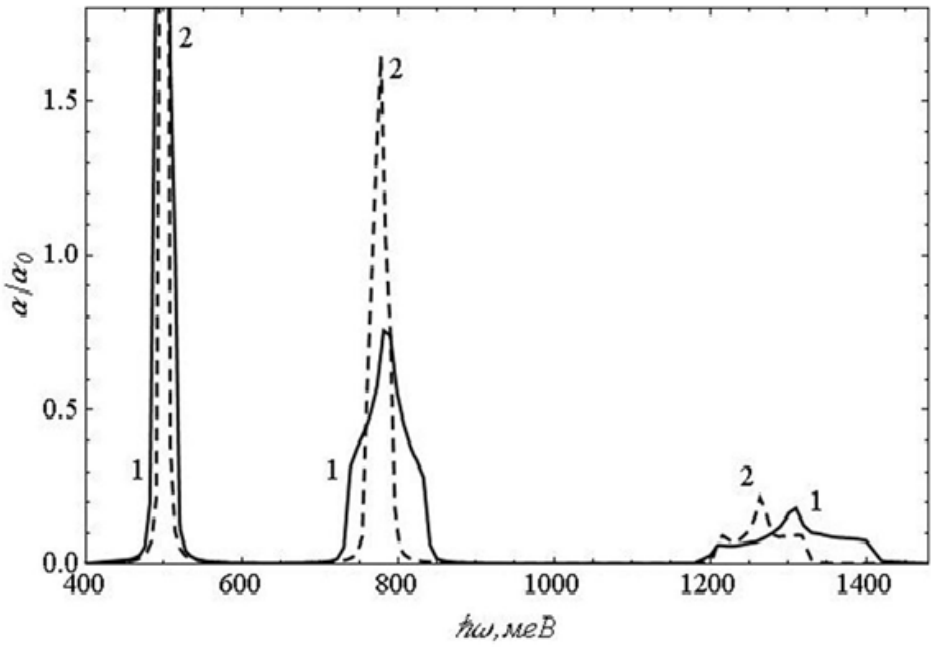

Fig.5. Light absorption coefficient in InAs/$In_{0.85}Ga_{0.15}As$ 2D-CQDS for L=96 Å at different interdot distances: d=12 Å (curve 1); d=24 Å (curve 2).

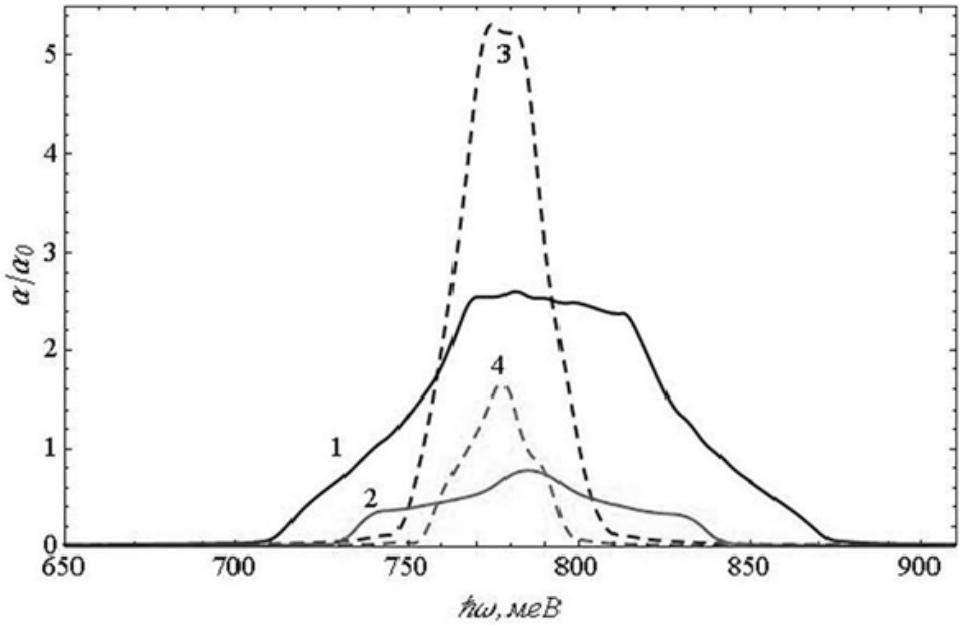

Fig.6. Light absorption coefficient in InAs/$In_{0.85}Ga_{0.15}As$ CQDS of various dimensionalities for L=96 Å at different interdot distances:
***d*=12 Å** 3D-CQDS (curve 1); 2D-CQDS (curve 2);
***d*=24 Å** 3D-CQDS (curve 3); 2D-CQDS (curve 4).

each of the present absorption bands.

Reducing of the dimensionality of the superlattice is obtained by significant increasing of the distance between the QDs in certain directions at constant sizes of quantum dots when tunneling of charges in these directions becomes impossible. Figure 5 shows the results of calculations of the absorption coefficient for the two-dimensional cubic quantum dot superlattice with dimensions L = 96 Å at different interdot distances d. As seen from the curves, a slight increase in the distance d from 12 Å (curve 1) to 24 Å (curve 2) reduces the width of the electron and hole subbands in a QD and results in narrowing of the range of photon frequencies of absorbed light. At the same time the peaks of the absorption bands are shifted towards lower frequencies with simultaneous increasing of absolute values of the absorption coefficient. This is also evident for the 3D-CQDS (curves 1,3 in Fig. 6). Here one of the three absorption regions (the central one) specific to a certain QD size (L = 96 Å) is chosen for the analysis. The comparison of absorption coefficients of different dimensionality superlattices is given in Fig. 6. For the 3D- (curves 1,3) and 2D- (curves 2,4) superlattices there is observed a narrowing of the absorption band with decreasing the dimensionality of the CQDS, and the invariance of the frequency of incident light, in which the absorption coefficient reaches its peaks. Figure 7 presents a complete pattern of dependences of the absorption

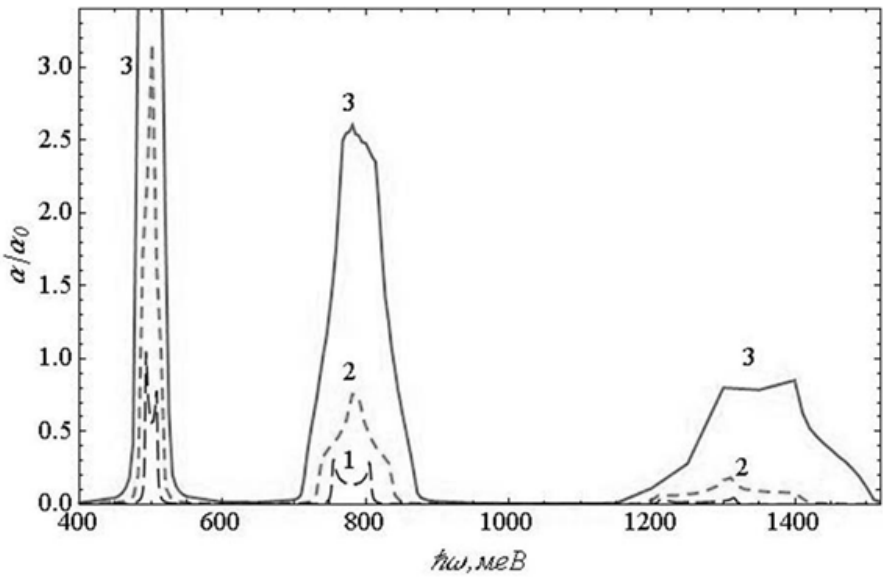

Fig.7. Light absorption coefficient in InAs/$In_{0.85}Ga_{0.15}As$ CQDS with L=96 Å, d=12 Å for various dimensionalities: 1D-CQDS (curve 1); 2D-CQDS (curve 2); 3D-CQDS (curve 3).

coefficient on the photon energy of the incident light for superlattices of all dimensionalities.

Conclusions

The results of our calculations of the interband absorption coefficient of the InAs/$In_{0.85}Ga_{0.15}As$ superlattice enable us to derive the following conclusions:

1. The absorption spectrum of the CQDS L = (60-100) Å is characterized by a pronounced peak and (depending on the QD size) one or two lower peaks shifted towards the short-wave region of the spectrum.
2. The dimensionality of the superlattice has influence on the shape of the absorption bands. The largest difference between the band shapes is observed for the 3D- and 1D-superlattices.
3. The increase in the distance between quantum dots is followed by narrowing of the absorption peaks for all three types of the superlattices.

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В.І. Бойчук, І.В. Білинський, Р.І. Пазюк

Коефіцієнт міжзонного поглинання світла надґраткою квантових точок $InAs/Ga_xIn_{1-x}As$ при низьких температурах

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У роботі розглянуто надґраткову систему $InAs/Ga_xIn_{1-x}As$ квантових точок малих розмірів (до 10 нм) кубічної форми. Для надграток різних вимірностей обчислено закони дисперсії для електронних та діркових підзон. Досліджено залежність коефіцієнта міжзонного поглинання від частоти світла, розмірів квантових точок та відстаней між ними. Показано, що вимірність надґратки впливає на форму смуг поглинання, збільшення відстані між квантовими точками спричиняє звуження піків поглинання для всіх трьох типів надґратки.

Ключові слова: квантова точка, надґратка, електронні стани, коефіцієнт поглинання.