

# THE INFLUENCE OF THE ELECTRICALLY INACTIVE IMPURITY ON THE ENERGY SPECTRUM OF ELECTRON AND HOLE IN InAs/GaAs HETEROSTRUCTURE WITH InAs QUANTUM DOTS

R. PELESHCHAK, O. KUZYK, O. DAN'KIV

Drohobych Ivan Franko State Pedagogical University,  
24, Ivan Franko Str., Drohobych, Ukraine

*E-mail:* rpeleshchak@ukr.net, olehkuzyk74@gmail.com, olesyadankiv16@gmail.com

*Received May 24, 2020*

*Abstract.* In the framework of electron-deformation model, the influence of the electrically inactive impurity on the energy spectrum of electrons and holes in InAs/GaAs heterostructure with InAs *quantum dots* (QD) is investigated. Two cases are considered: the isovalent impurity of substitution and the neutral atom in the internode. It is established that the presence of the impurity in the center of spherical quantum dot leads to a decrease in energy of radiation, which corresponds to the recombination transition between the ground states of electron and hole. This effect is better manifested for small quantum dots and in the presence of interstitial impurity.

*Key words:* quantum dot, isovalent impurity, deformation, energy of electron and hole.

## 1. INTRODUCTION

Future progress in the development of heterolasers is connected with the application of structures with QDs in their active region [1–11]. Semiconducting heterostructures InAs/GaAs with InAs QDs have a high quantum yield of photoluminescence, being a promising material for the creation of lasers is the near infrared spectral region [1, 2, 4–6].

One method to control the physical parameters of InAs/GaAs heterostructures with QDs is to introduce impurities into their active area [2, 5, 10, 11]. In recent years, a new approach to controlling the properties of semiconductor *quantum dot* (QD) heterostructures has been developed. The approach is based on the introduction of a single impurity atom into a QD [12]. This problem is prospective for present day optoelectronics, specifically, for the production of single electron devices that may find application in quantum computers [13, 14]. The extraordinary properties of QD structures reveal themselves, only if the QDs are as uniform in size and shape as possible and the QD array is of high density (about  $10^{11}$  cm<sup>-2</sup>). Therefore, the main problem in growing QDs is to control their morphology: the average size, density, uniformity, etc. All of these QD characteristics can be controlled by

varying the technological parameters of the growth process [15, 16]. Another approach to controlling the properties of QD semiconductor heterostructures is based on the introduction of a single impurity atom into a QD [12, 14]. Isovalent doping of single crystal materials is an important technique for solving many practical problems.

In works [2, 5, 10, 11], it was found experimentally that the introduction of stibium [2], nitrogen [5, 10], and bismuth [11] impurities considerably improves the optical properties of InAs/GaAs QDs. In work [11], the theory of deformation was developed for QDs doped with isovalent impurity. The theory explained experimental data on the creation of an array of uniform InAs QDs doped with Bi [17]. Bismuth is not an electrically active impurity, *i.e.* it does not increase the charge carrier concentration. However, it substantially changes the conditions of QD formation owing to the induced diffusion-deformation flux. It has also been shown in experimental work [2, 5, 10] that the introduction of nitrogen and stibium impurities enhances the optical properties of InAs/GaAs QDs. These impurities are also isovalent to As. The change in optical properties is explained by the fact that the impurities of nitrogen or Sb reduce the mechanical stress that arises at the expense of the mismatch of the lattice parameters of the InAs and GaAs.

Although isovalent impurities do not change the concentration of charge carriers, they can change the band structure of quantum dots. This is mainly due to the fact that the impurities are centers of deformation, which leads to the local shift of the bottom of the conduction band (the vertices of the valence band). And this in turn leads to the change in the energy of electron and hole and, accordingly, the energy of the quantum that is emitted, such as the energy of recombination radiation [18]. Thus, the study of the influence of isovalent doping of InAs/GaAs QDs on the energy spectrum of electrons and holes is an urgent problem. In this paper, we construct the theoretical model of the influence of deformation, created by neutral impurity, on the energy of recombination radiation, which corresponds to the transition between the ground states of electron and hole in the InAs/GaAs heterostructure with the InAs QDs.

## 2. THE DEFORMATION OF THE InAs/GaAs QUANTUM DOT WITH IMPURITY

In the system of strained InAs islands, there exist two sources of the elastic strain fields: on the one hand, there is a lattice mismatch between the QD and substrate materials ( $f = (a^{\text{InAs}} - a^{\text{GaAs}}) / a^{\text{InAs}} \approx 7\%$ ) and, on the other hand, there is a step in the surface tension tensor at the island edges. Correspondingly, the elastic energy is equal to the sum of the energy of elastic relaxation in the bulk, the energy of elastic relaxation at the island edges, and the energy of interaction of the two elastic fields [19]. In this study, we consider QDs that do not exhibit any well pronounced crystallographic faceting. Specifically, we consider QDs, whose shape corresponds to almost spherical symmetry. For example, in the InAs/GaAs(001)

heterosystem, such QDs are formed at thicknesses of the growing InAs layer of about 2 ML [20]. Therefore, in what follows, the contribution of the island edges to the energy of elastic relaxation is disregarded.

In order to reduce the problem for a large number of QDs to that for one QD, we use the following approximation: the energy of pairwise interaction between QDs is replaced by the energy of interaction of each QD with the averaged (effective) field of elastic stresses  $\sigma_{eff}$  of all other QDs [11]. Let us consider a spherical QD of radius  $R_0$  embedded into a semiconductor matrix of radius  $R_1$ . Let us assume that the isovalent impurity is located at the center of the sphere.

To determine the strain tensor components, we must determine the explicit form of the atomic displacements and in the InAs and GaAs materials, respectively. For a QD with an implanted impurity, the equilibrium equation is [21]

$$\bar{\nabla} \operatorname{div} \bar{u} = -D_1 \cdot \bar{F}^{(1)}(\bar{r}), \quad (1)$$

$$D_1 = \frac{(1 + \nu_1)(1 - 2\nu_1)}{E_1(1 - \nu_1)}; \quad \bar{F}^{(1)} = \frac{2\Delta\Omega}{3\pi^{3/2}} (C_{11}^{(1)} + 2C_{12}^{(1)}) \frac{1}{r_0^5} r e^{-\frac{r^2}{r_0^2}} \bar{n}; \quad \bar{n} = \bar{r}/|\bar{r}|,$$

where  $\bar{F}^{(1)}$  is the volumetric force produced by the impurity in the QD;  $\Delta\Omega$  is the change in the volume of the QD material due to the embedded isovalent impurity;  $r_0$  is the effective radius of the impurity atom; and  $\nu_i$ ,  $E_i$  are, correspondingly, the Poisson coefficients and the Young moduli of the QD material and the surrounding matrix. The parameters  $\nu_i$  and  $E_i$  can be expressed in terms of the elastic constants  $C_{11}^{(i)}$  and  $C_{12}^{(i)}$  of these materials in a well known manner [21].

In the following we will consider two cases: 1) the isovalent impurity ion ( $\text{Bi}^{3+}$ ,  $\text{Sb}^{3+}$ ) substitutes a host  $\text{As}^{3+}$  ion; 2) the neutral impurity occupies an interstitial position in the InAs semiconductor material. The effective radius of the impurity atom  $r_0$  is equal to the ion radius  $r_i$  when it substitutes the atom in the node of the crystal lattice. In the second case, when the impurity is in the interstice,  $r_0 = a^{(1)}$  ( $a^{(1)}$  is the parameter of the crystal lattice of the QD) [22]. The change  $\Delta\Omega$  in the volume of the QD in these two cases is determined by formulas [22]:

1) for impurity of substitution:

$$\Delta\Omega = 4\pi(r_i^3 - r_{\text{As}}^3)/3, \quad (2)$$

2) for atom in the internode:

$$\Delta\Omega = 4\pi r_a^3/3, \quad (3)$$

where  $r_{\text{As}}$ ,  $r_a$  are the  $\text{As}^{3+}$  ion radius and the radius of the impurity atom.

In the spherical coordinates, the solution of Eq. (1) is

$$u_r^{(1)} = C_1 r + C_2 / r^2 - AD_1 r_0^4 e^{-r^2/r_0^2} / 4r + AD_1 \sqrt{\pi} r_0^5 \text{Erf}(r/r_0) / 8r^2, \quad 0 \leq r \leq R_0, \quad (4)$$

where  $A = 2\Delta\Omega\pi^{-3/2}(C_{11}^{(1)} + 2C_{12}^{(1)}) / 3r_0^5$ .

Since the displacement at the point  $r = 0$  must be finite, we must set  $C_2 = 0$  in the solution (4).

The atomic displacement in the GaAs matrix is

$$u_r^{(2)} = C_3 r + C_4 / r^2, \quad R_0 \leq r \leq R_1. \quad (5)$$

The components of the strain tensors for the QD and matrix materials are

$$\varepsilon_{rr}^{(i)} = \partial u_r^{(i)} / \partial r, \quad \varepsilon_{\theta\theta}^{(i)} = \varepsilon_{\varphi\varphi}^{(i)} = u_r^{(i)} / r, \quad \varepsilon^{(i)} = Sp\varepsilon^{(i)} = \varepsilon_{rr}^{(i)} + \varepsilon_{\theta\theta}^{(i)} + \varepsilon_{\varphi\varphi}^{(i)}. \quad (6)$$

Then from (4) – (6) we get:

$$\varepsilon^{(1)} = 3C_1 + AD_1 r_0^2 e^{-r^2/r_0^2} / 2, \quad (7)$$

$$\varepsilon^{(2)} = 3C_3. \quad (8)$$

The coefficients  $C_1$ ,  $C_3$ , and  $C_4$  can be determined by solving the system of boundary conditions

$$\begin{cases} 4\pi R_0^2 \left( u_r^{(2)} \Big|_{r=R_0} - u_r^{(1)} \Big|_{r=R_0} \right) = \Delta V, \\ \sigma_{rr}^{(1)} \Big|_{r=R_0} = \sigma_{rr}^{(2)} \Big|_{r=R_0} - P_L, \\ \sigma_{rr}^{(2)} \Big|_{r=R_1} = \sigma_{ef}. \end{cases} \quad P_L = \frac{2\gamma(\varepsilon^{(1)})}{R_0} \quad (9)$$

The first equation of system (9) expresses the mismatch between the lattice parameters of the contact materials [18],  $\Delta V = f \cdot 4\pi R_0^3$ ;  $P_L$  is the Laplace pressure; and  $\gamma(\varepsilon^{(1)})$  is the surface energy of the InAs QD. This surface energy is a function of the surface stress and strain of the QD [23].

The stresses  $\sigma_{rr}^{(i)}$  in the QD and matrix materials are determined as [24]:

$$\sigma_{rr}^{(i)} = \frac{E_i}{(1 + \nu_i)(1 - 2\nu_i)} \left[ (1 - \nu_i) \varepsilon_{rr}^{(i)} + \nu_i (\varepsilon_{\varphi\varphi}^{(i)} + \varepsilon_{\theta\theta}^{(i)}) \right]. \quad (10)$$

### 3. THE POTENTIAL ENERGY OF ELECTRON AND HOLE IN THE InAs/GaAs QUANTUM DOT WITH ISOVALENT IMPURITY

In the case of heterostructures with strained QDs, the depth of the quantizing potential is determined by both the internal deformation in the contacting QD and matrix materials, which arises owing to the mismatch between the lattice parameters in them, and the deformation induced by the impurity.

The shifts of the edges of both allowed energy bands as a result of elastic straining can be expressed:  $\Delta E_c^{(i)}(t) = a_{c,v}^{(i)} \varepsilon^{(i)}$  ( $a_c^{(i)}$  ( $a_v^{(i)}$ ) are the constants of the hydrostatic deformation potential of the conduction (valence) bands).

Hence, the potential energies  $W^{(e,h)}(r)$  of electron and hole in the strained InAs/GaAs heterosystem with spherical InAs QDs are

$$W^{(e,h)}(r) = \begin{cases} -V_0^{(e,h)} e^{-r^2/r_0^2}, & 0 \leq r \leq R_0 \\ V_2^{(e,h)}, & R_0 \leq r \leq R_1 \end{cases}, \quad (11)$$

where  $V_0^{(e,h)} = |a_{c,v}^{(1)}| AD_1 r_0^2 / 2$ ,  $V_2^{(e,h)} = \Delta E_{c,v}(0) + 3|a_{c,v}^{(1)}| C_1 - |a_{c,v}^{(2)}| \varepsilon^{(2)}$ ;  $\Delta E_{c,v}(0)$  is the depth of potential wells for electron and hole in an unstrained QD,

$$\Delta E_c(0) = \chi_1 - \chi_2; \quad \Delta E_v(0) = E_g^{(2)}(0) + \chi_2 - E_g^{(1)}(0) - \chi_1; \quad (12)$$

$\chi_i$ ,  $E_g^{(i)}(0)$  are the electron affinity and the energy gap width InAs ( $i = 1$ ) and GaAs ( $i = 2$ ) unstrained material. The energy is reckoned from the edge of the corresponding allowed band in InAs without impurity.

In Fig. 1 shows the coordinate dependence of the potential energy of electron and hole in the GaAs/InAs QDs containing the neutral atom N (4), P (3) in the interstitial or the isovalent impurity ion  $\text{Sb}^3$  (2),  $\text{Bi}^{3+}$  (1) substituting a host  $\text{As}^{3+}$  ion. As a rule, impurities with the larger ionic radius are impurities of substitution, and impurities with the smaller ionic radius are located in the internode [22]. The calculations were carried out using the following parameters [23, 25, 26, 27]:  $\chi_1 = 4.9 \text{ eV}$ ;  $\chi_2 = 4.07 \text{ eV}$ ;  $a_c^{(1)} = -5.08 \text{ eV}$ ;  $a_c^{(2)} = -7.17 \text{ eV}$ ;  $a_v^{(1)} = 1 \text{ eV}$ ;  $a_v^{(2)} = 1.16 \text{ eV}$ ;  $E_g^{(1)}(0) = 0.36 \text{ eV}$ ;  $E_g^{(2)}(0) = 1.45 \text{ eV}$ ;  $m_1^{(e)} = 0.057 m_0$ ;  $m_2^{(e)} = 0.065 m_0$ ;  $m_1^{(h)} = 0.41 m_0$ ;

$m_2^{(h)} = 0.45 m_0$ ;  $C_{11}^{(1)} = 0.83$  Mbar;  $C_{12}^{(1)} = 0.45$  Mbar;  $C_{11}^{(2)} = 1.22$  Mbar;  $C_{12}^{(2)} = 0.57$  Mbar;  $\gamma = 0.57$  N/m;  $\sigma_{ef} = 10^9$  N/m<sup>2</sup>;  $R_1 = 50$  nm.

Calculations are presented for quantum dots with the radius of 2 nm. For other QD sizes, the picture does not change qualitatively. The presence of the impurity leads to the decrease in the potential energy in the center of the quantum dot, which is explained by the character of the distribution of deformation.

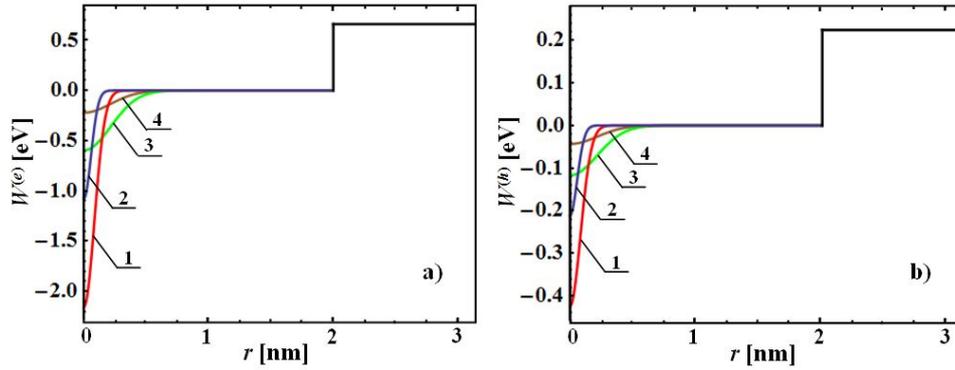


Fig. 1 – (Color online) The coordinate dependence of the potential energy of electron (a) and hole (b) in the InAs/GaAs quantum dot with the isovalent impurity Bi<sup>3+</sup> (curve 1), Sb<sup>3+</sup> (curve 2) or the internodal atom P (curve 3), N (curve 4).

In both cases, the impurity is the center of stretching, and the strain reverses its character in the vicinity of the impurity. With increasing distance from the QD center, the hydrostatic compressive strain of the QD material steadily increases to a value that is virtually no different from that of the impurity free QD material, in which the compressive strain is caused by the lattice mismatch between the contacting materials. In case of impurity of substitutes (curves 1 and 2), the stretching strain produced in the vicinity of the impurity is higher in magnitude and more localized around the QD center. This is attributed to the much smaller effective range of elastic action of a substitutional defect in comparison to that of an interstitial atom.

#### 4. THE ENERGY SPECTRA OF ELECTRONS AND HOLES IN THE STRAINED InAs/GaAs HETEROSYSTEM WITH SPHERICAL InAs QDs WITH ISOVALENT IMPURITY

The energy spectra are determined by solving the Schrödinger equation

$$\hat{H}_{e,h} \Psi^{(e,h)}(r, \theta, \varphi) = E^{(e,h)} \Psi^{(e,h)}(r, \theta, \varphi) \quad (13)$$

with the Hamiltonian

$$\hat{H}_{e,h}(r, \theta, \varphi) = -\frac{\hbar^2}{2} \vec{\nabla} \frac{1}{m^{(e,h)}} \vec{\nabla} + W^{(e,h)}(r). \quad (14)$$

The Schrödinger equation (13) with the Gaussian potential (11) is not solved analytically. Various approaches to finding approximate solutions have been proposed in [28 – 30]. All the presented methods are approximate and are used for the infinite area ( $r \rightarrow \infty$ ).

To find the solution of Schrödinger equation (13), the following procedure was performed:

1) the potential (11) was approximated as

$$W_1^{(e,h)}(r) = \begin{cases} -V_0^{(e,h)} \left(1 - r^2 / r_c^2\right), & 0 \leq r \leq r_c \\ 0, & r_c \leq r \leq R_0 \\ V_2^{(e,h)}, & R_0 \leq r \leq R_1 \end{cases} \quad (15)$$

2) the parameter  $r_c$  was found from the condition of the minimum of functional  $f(k) = \int_0^{r_c} \left(-V_0^{(e,h)} e^{-r^2/r_0^2} + V_0^{(e,h)} \left(1 - r^2 / r_c^2\right)\right)^2 dr + \int_{r_c}^{R_0} \left(-V_0^{(e,h)} e^{-r^2/r_0^2}\right)^2 dr$

3) the Schrödinger equation with potential (15) was solved, from which the energy of electron and hole  $E_{nl}^{(e,h)}$  was found in the zero approximation;

4) the perturbation theory was used and in the first approximation the corrections to the energies of electron (hole) are calculated by the formula

$$\Delta E_{nl}^{(e,h)} = \int_V \Psi_{nlm}^{*(e,h)}(\vec{r}) \Delta V^{(e,h)}(r) \Psi_{nlm}^{(e,h)}(\vec{r}) d^3 \vec{r}, \quad (16)$$

where  $\Delta V^{(e,h)} = W^{(e,h)} - W_1^{(e,h)}$ .

The solution of the Schrödinger equation (13) has the form

$$\Psi_{nlm}^{(e,h)}(r, \theta, \varphi) = R_{nl}^{(e,h)}(r) \cdot Y_{lm}^{(e,h)}(\theta, \varphi), \quad (17)$$

where  $Y_{lm}^{(e,h)}(\theta, \varphi)$  are the spherical Legendre functions. The radial functions  $R_{nl}^{(e,h)}(r) = \rho_{nl}^{(e,h)}(r)/r$  are expressed in terms of the confluent hypergeometric function and the spherical Bessel functions ( $0 \leq E_{nl}^{(e,h)} \leq V_2^{(e,h)}$ ):

$$\rho_{1nl}^{(e,h)}(r) = B_1^{(e,h)} r^{l+1} e^{-\lambda^{(e,h)} r^2 / 2} {}_1F_1\left(l/2 + 3/4 - \mu^{(e,h)} / 2, l + 3/2, \lambda^{(e,h)} r^2\right) \quad 0 \leq r \leq r_c \quad (18)$$

$$\rho_{2nl}^{(e,h)}(r) = B_2^{(e,h)} \cdot j_l(k_{2e,h}r) + B_3^{(e,h)} \cdot n_l(k_{2e,h}r), \quad r_c \leq r \leq R_0 \quad (19)$$

$$\rho_{3nl}^{(e,h)}(r) = B_4^{(e,h)} \cdot h_l^{(1)}(ik_{3e,h}r) + B_5^{(e,h)} \cdot h_l^{(2)}(ik_{3e,h}r), \quad R_0 \leq r \leq R_1 \quad (20)$$

where  $\lambda^{(e,h)} = \sqrt{2m_1^{(e,h)}V_0^{(e,h)} / \hbar r_c}$ ,  $\mu = k_{1e,h}^2 / \lambda$ ,  $k_{1e,h}^2 = 2m_1^{(e,h)}(E_{nl}^{(e,h)} + V_0^{(e,h)}) / \hbar^2$ ,  $k_{2e,h}^2 = 2m_1^{(e,h)}E_{nl}^{(e,h)} / \hbar^2$ ,  $k_{3e,h}^2 = 2m_2^{(e,h)}(V_2^{(e,h)} - E_{nl}^{(e,h)}) / \hbar^2$ .

In (18) the condition of regularity of the function  $R_{nl}^{(e,h)}(r)$  at  $r \rightarrow 0$  is taken into account. The continuity conditions for the wave functions and density of the flow of probability at the QD-matrix interface,

$$\begin{cases} R_{1nl}^{(e,h)}(r)|_{r=r_c} = R_{2nl}^{(e,h)}(r)|_{r=r_c}, \\ dR_{1nl}^{(e,h)}(r)/dr|_{r=r_c} = dR_{2nl}^{(e,h)}(r)/dr|_{r=r_c}, \\ R_{2nl}^{(e,h)}(r)|_{r=R_0} = R_{3nl}^{(e,h)}(r)|_{r=R_0}, \\ m_1^{(e,h)-1} dR_{2nl}^{(e,h)}(r)/dr|_{r=R_0} = m_2^{(e,h)-1} dR_{3nl}^{(e,h)}(r)/dr|_{r=R_0} \end{cases} \quad (21)$$

along with the regularity condition of the functions  $R_{nl}^{(e,h)}(r)$  at  $r \rightarrow R_1$  and with normalization determine the energy spectrum  $E_{nl}$  and wave functions of electron and hole in the InAs/GaAs heterosystem with the InAs QDs.

Figures 2 show the (a) electron and (b) hole energies in the ground states plotted *versus*  $R_0$  for InAs QDs in a GaAs. As can be seen, an increase in the QD size is accompanied by a monotonic decrease in the electron and hole energy levels. The presence of isovalent impurities leads to the decrease in the energy of electron and hole. This is especially true for quantum dots of smaller sizes. Thus, at  $R_0 = 2$  nm, the energy of electron in the quantum dot with impurity of phosphorus is reduced by 60 meV compared to the QD without impurities. The change in the energy of electron and hole is more significant in the presence of impurities in the internode (P, N). In particular, at  $R_0 = 2$  nm, the energy of electron in the quantum dot with the  $\text{Sb}^{3+}$  impurity of substitution decreases only by 9 meV compared to the QD without impurities. Such regularities are explained by the type of potential energy for these impurities (Fig. 1). The additional potential well, created by isovalent impurities of substitution ( $\text{Bi}^{3+}$ ,  $\text{Sb}^{3+}$ ) is deeper, but very narrow.

The radiation energy, which corresponds to the recombination transition between the ground states of electron and hole in a InAs QD, can be determined:

$$E_0 = E_{10}^{(e)} + E_{10}^{(h)} + E_g^{(1)}(\varepsilon) = E_{10}^{(e)} + E_{10}^{(h)} + E_g^{(1)}(0) + 3(a_c^{(1)} - a_v^{(1)})C_1. \quad (22)$$

In [2, 5, 10] it is noted that the disadvantage of the InAs/GaAs QDs is the increase in the width of the optical gap (the distance between the ground states of electron and hole) due to the significant mismatch of the lattice parameters of InAs and GaAs. This increase is due to the deformation shift of the edges of the permitted bands (the last term in formula (22)). The introduction of impurities, which are the centers of stretching, allows to some extent to compensate for the deformation of compression due to the mismatch of contacting lattices. In Fig. 3 shows the dependence of the radiation energy, which corresponds to the recombination transition between the ground states of electron and hole in the InAs QD, from QD radius in the presence and absence of impurities.

As you can see from Fig. 3, the introduction of isovalent impurities leads to the decrease in the energy of recombination radiation. The best effect is created by internodal impurities. In particular, in the presence of phosphorus and nitrogen impurities in the quantum dot with radius of 2 nm, the energy of recombination radiation decreases by 85 meV and 57 meV, respectively. The obtained results qualitatively coincide with the experimental data of works [2, 5, 10].

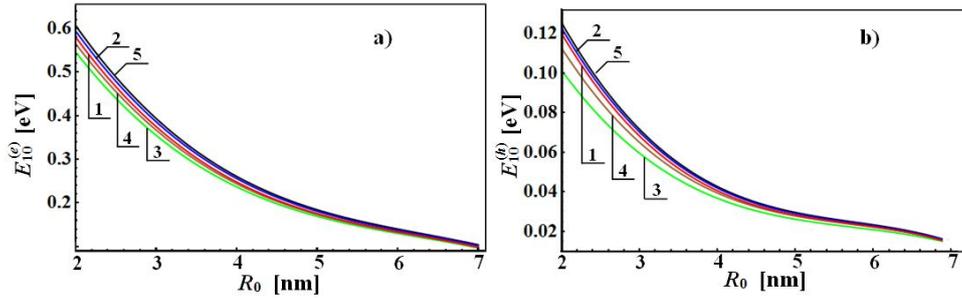


Fig. 2 – (Color online) Dependence of the energy of electron (a) and hole (b) in the ground state on QD radius  $R_0$  for the InAs/GaAs heterosystem with isovalent impurity of substitution  $\text{Bi}^{3+}$  (1),  $\text{Sb}^{3+}$  (2) or internodal atom P (3), N (4) and without impurity (5).

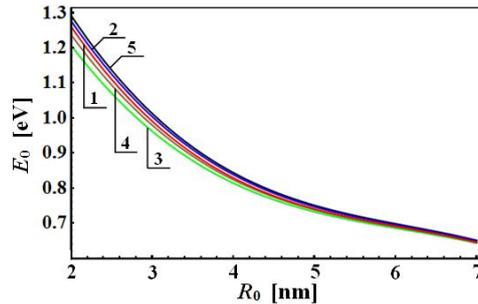


Fig. 3 – (Color online) Dependence of the energy of recombination radiation on QD radius for the InAs/GaAs heterosystem with isovalent impurity of substitution  $\text{Bi}^{3+}$  (curve 1),  $\text{Sb}^{3+}$  (curve 2) or internodal atom P (curve 3), N (curve 4) and without impurity (curve 5).

## 5. CONCLUSIONS

In this work, the deformation model of the InAs/GaAs heterostructure with InAs quantum dots, containing the electrically inactive impurity in the center of the quantum dot, is constructed. The impurity may be in the internode or substitute the As<sup>3+</sup> in the node. In both cases, the impurities are centers of stretching, because only isovalent impurities with the larger ionic radius (Bi<sup>3+</sup>, Sb<sup>3+</sup>) are considered at the substitution. Within the framework of the developed model, the deformation of InAs/GaAs heterostructure materials is calculated. The deformation is created both due to the mismatch of the lattice parameters of crystalline materials and impurities.

The regularities of the change of the energy spectrum of electron and hole during the introduction of the single electrically inactive impurity into the quantum dot (the isovalent impurities of substitution Bi<sup>3+</sup>, Sb<sup>3+</sup> or the neutral interstitial atoms N and P) at different radii of spherical quantum dots have been investigated. It is established that the presence of such impurities leads to the decrease in the ground energy states of electron and hole and, accordingly, to the decrease in the energy of recombination radiation. This effect is more significant for smaller quantum dots. This can be explained by their greater sensitivity to deformation.

## REFERENCES

1. N.N. Ledentsov, *Semicond. Sci. Technol.* **26**, 014001 (2011).
2. C. Zhou, B. Liang, J. Liu, Y. Wang, Y. Guo, S. Wang, G. Fu, *Optical Mater.* **98**, 109479 (2019).
3. M. Tkach, R. Fartushinsky, J. Seti, *Rom. J. Phys.* **55**, 93-101 (2010).
4. E. Stock, M.-R. Dachner, T. Warming, A. Schliwa, *Phys. Rev. B* **83**, 041304 (2011).
5. S. Naceur, M. Choubani, B. Smiria, H. Maarefa, G. Monierb, *Vacuum* **172**, 109097 (2020).
6. R.M. Peleshchak, O.V. Kuzyk, O.O. Dan'kiv, *Physica E: Low-dimensional Systems and Nanostructures* **119**, 113988 (2020).
7. R.M. Peleshchak, O.V. Kuzyk, O.O. Dan'kiv, *J. Nano- and Electronic Phys.* **8**, 02014 (2016).
8. R.M. Peleshchak, O.V. Kuzyk, O.O. Dan'kiv, *Journal of Nano Research* **57**, 40 (2019).
9. R.M. Peleshchak, O.O. Dan'kiv, O.V. Kuzyk, *Ukr. J. Phys.* **57**, 68 (2012).
10. M.O. Valappil, J. Mohamed S, S. Alwarappa, *Materials Research Express*, **7**, 014005 (2020).
11. R.M. Peleshchak, S.K. Guba, O.V. Kuzyk, I.V. Kurilo, O.O. Dan'kiv, *Semiconductors* **47**, 349 (2013).
12. L.E. Vorob'ev, V.Yu. Panevin, N.K. Fedosov, D.A. Firsov, *Semiconductors* **39**, 50 (2005).
13. V.V. Svetukhin, S.V. Bulyarskii, D.V. Sanchishchin, *Technical Phys. Lett.* **30**, 220 (2004).
14. J.R. Weber, W.F. Koehl, J.B. Varley, *Proceed. National Academy Scien.* **107**, 8513 (2010).
15. V.A. Osipov, F. Schenitt, S.A. Kukushkin, P. Hess, *Appl. Surf. Sci.* **188**, 156 (2002).
16. V.G. Dubrovskii, G.E. Cirlin, V.M. Ustinov, *Phys. Rev. B* **68**, 075409 (2003).
17. N. Zvonkov, I.A. Karpovich, N.V. Baidus', D.O. Filatov, *Semiconductors* **35**, 93 (2001).
18. B.V. Novikov, G.G. Zegrya, R.M. Peleshchak, O.O. Dan'kiv, *Semiconductors* **42**, 1076 (2008).
19. V.A. Shchukin, N.N. Ledentsov, P.S. Kop'ev, D. Bimberg, *Phys. Rev. Lett.* **75**, 2968 (1995).
20. Z.M. Wang, K. Holmes, Yu.I. Mazyr, G.J. Salamo, *Appl. Phys. Lett.* **84**, 1931 (2004).
21. K. Teodosiu, *Elastic Models of Crystal Defects*, Springer, Berlin, Heidelberg, New York, 1982.
22. A.M. Kosevich, *The Crystal Lattice*, Wiley-VCH Verlag GmbH & Co. KGaA, 2005.

23. N. Moll, M. Scheffler, E. Pehlke, Phys. Rev. B **58**, 4566 (1998).
24. L.D. Landau, E.M. Lifshitz, *Theory of elasticity*, Pergamon Press, London, 1970.
25. Chris G. Van de Walle, Phys. Rev. B **39**, 1871 (1989).
26. A. Qteish and R.J. Needs, Phys. Rev. B **45**, 1317 (1992).
27. R.M. Peleshchak, O.V. Kuzyk, O.O. Dan'kiv, Ukr. J. Phys. **61**, 741 (2016).
28. H. Mutuk, Pramana – J. Phys. **92**, 66 (2019).
29. G. Stephenson, Journal of Physics A: Mathematical and General **10**, L229 (1977).
30. E. Omugbe, O.E. Osafire, E.A. Enaibe, International Res. J. Pure and Appl. Phys. **6**, 1 (2019).