Influence of impurity on electronic transition in coherent-strained quantum dot

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The influence of impurity on energy breadth of an optical gap for quantum dot is studied within the framework of deformation potential model. It is established that with size increase of a quantum dot with an ionization donor dopant an optical gap diminishes. For smaller radiuses ($R_0 \sim 40$ Å $\div 57$ Å) energy breadth of the basic optical transition E in quantum dots with donor dopants is greater, than in unblended ones. For the major sizes of quantum dots $R_0 \geq 58$ Å the converse effect is observed.

В рамках модели деформационного потенциала исследовано влияние примеси на энергетическую ширину оптической щели квантовой точки. Установлено, что с увеличением размеров квантовой точки с ионизированной донорной примесью оптическая щель суживается. Для меньших радиусов ($R_0 \sim 40$ Å $\div 57$ Å) энергетическая ширина основного оптического перехода E в квантовых точках с донорными примесями больше, чем без примесей. При больших размерах квантовых точек $R_0 \geq 58$ Å наблюдается обратный эффект.

Optical properties of heterostructures with InAs small-sized quantum dots (about several nanometers) are actively studied in order to create solid-state emitters in the range $\lambda \sim 1.4$ μm.

One of the promising ways to control the emission range is introduction of unit impurity atom into the quantum dot (QD) [1, 2]. The technology of impurity atom introducing into the QD is based on the union of heterosystem growth process with quantum dots (by molecular-radiation epitaxy) and selective doping [3]. This problem is of scientific as well as of practical interest for modern optoelectronics, in particular, for optoelectronic devices applicable in quantum computers [4]. In this light, the estimates of the basic optical transition energy in strained nanoheterosystems with QD in the presence of impurities and the analysis of this energy (or frequency) dependence on quantum dot size as well as on the impurity type are helpful.

The experimental study of optic phenomena in the InAs/GaAs heterosystems with doped QD was carried out in the work [2]. The spectra of a quasiparticle moving in the superposition of fields with Coulomb and radial rectangular potential, the forces of the fields having shared centres, was theoretically studied in the framework of dielectric formalism [5, 6].

In this paper, we are going to calculate the size of optical gap for InAs coherent-strained spherical QD doped with silicon and to analyze the dependence of this energy shift on the QD size, taking into account the deformation potential.

Let us consider spherical InAs QD with radius R_0 and inductivity ε_1, placed into a semiconductor GaAs matrix with radius R_1 and inductivity ε_2. There is ionized donor Si impurity with charge $+e$ in InAs QD centre.

In order to reduce the problem with a number of QD to a problem with one QD, we take the following approximation: we sub-

stitute the pair-wise elastic interaction energy of the quantum dots by the interaction energy of every QD with averaged elastic deformation field $\sigma_{ef}(N-1)$ of the rest of QD's.

Unlike [7, 8], our InAs/GaAs (with InAs QD) heterostructure model takes into account the influence of internal elastic stresses, caused by the disagreement in the QD lattice material parameters and the matrix $f = a^{InAs} - a^{GaAs}/\quad a^{InAs} \approx 7~\%$, Laplacian pressure on the boundary between QD and the matrix (considering self-consistent deformation of QD material and surrounding finite-sized matrix), the difference in physical characteristics of nanoobjects and massive crystals (baric coefficient, modulus of elasticity, Poisson's ratio), as well as electron deformation interaction.

As the lattice constant of InAs material is more than that of GaAs matrix, then in case of heteroepitaxial growth within pseudomorphous InAs growth on GaAs layer, InAs material can be deformed by compression and GaAs — by stretching. So, we introduce the spherical quantum dot with radius R_0, charged by donor impurity, as an elastic dilatation microinclusion in the form of an elastic ball placed into a spherical empty space with the volume ΔV smaller than the volume of the microinclusion, in the GaAs matrix. To insert such a spherical microinclusion, one should squeeze it and stretch the GaAs matrix in the radial directions. The simultaneous deformation result for the contacting nanomaterials is described by ΔV volume change with the parameter $f(R_0, R_1)$:

$$\Delta V(R_0, R_1) = f(R_0, R_1) \cdot 4\pi R_0^3. \qquad (1)$$

Unlike [8, 9], in our paper the disagreement parameter $f(R_0, R_1)$ is the function of sizes QD (R_0) and the radius if the surrounding matrix (R_1):

$$f(R_0, R_1) = f_1(R_0, R_1) + f_2(R_0, R_1), \qquad (2)$$

where $f_1(R_0, R_1)$, $f_2(R_0, R_1)$ are materials of QD and the surrounding matrix lattice parameters relative changes, caused respectively by the difference of radial $a_r^{(i)}$ and angle constituents $a_\theta^{(i)}$, $a_\varphi^{(i)}$ of lattice parameter in QD material as well as in the surrounding matrix, relative to their values a_i in bulk materials InAs and GaAs,

$$f_i(R_0, R_1) = \frac{1}{3a_i}\left(2a_\theta + a_r^{(i)}\right) - 1, \qquad (3)$$

$$a_\theta = a_\varphi = \frac{a_1 G_1 R_0 + a_2 G_2 (R_1 - R_0)}{G_1 R_0 + G_2 (R_1 - R_0)};$$

$$a_r^{(i)} = a_i\left(1 - D_{001}^{(i)} \cdot \left(\frac{a_\theta}{a_i} - 1\right)\right);$$

$$D_{001}^{(i)} = 2\frac{C_{12}^{(i)}}{C_{11}^{(i)}};$$

$C_{11}^{(i)}$, $C_{12}^{(i)}$ are elastic constants of InAs ($i = 1$) and GaAs ($i = 2$) materials; G_1; G_2 are modulus of rigidity for the materials InAs and GaAs.

As $R_1/R_0 \gg 1$, then $f_2/f_1 \ll 1$.

The strain $\sigma_{rr}^{(i)}$ in the materials InAs and GaAs is [10]:

$$\sigma_{rr}^{(i)} = \frac{E_i}{(1 + \nu_i)(1 - 2\nu_i)} \times \qquad (4)$$

$$\times \left[(1 + \nu_i)\varepsilon_{rr}^{(i)} + \nu_i(\varepsilon_{\varphi\varphi}^{(i)} + \varepsilon_{\theta\theta}^{(i)})\right],$$

where ν_i, E_i are Poisson's ratio and modulus of elasticity for the materials of QD and the surrounding matrix, expressed in the known way [10] by the elastic constants of these materials.

To clear out the components of deformation tensor, we need to find the explicit form of atoms shift $u_r^{(1)}$, $u_r^{(2)}$ in InAs and GaAs materials, respectively. To do it, let us write down the equilibrium equation [11]:

$$\nabla \text{div}\mathbf{u} = 0 \qquad (5)$$

with the following edge conditions for spherical QD:

$$\begin{cases} 4\pi R_0^2\left(u_r^{(2)}\big|_{r=R_0} - u_r^{(1)}\big|_{r=R_0}\right) = \Delta V, & (6) \\[2mm] \sigma_{rr}^{(1)}\big|_{r=R_0} = \sigma_{rr}^{(2)}\big|_{r=R_0} + P_L, \quad P_L = \frac{2\alpha(\varepsilon^{(1)})}{R_0} \\[2mm] \sigma_{rr}^{(2)}\big|_{r=R_1} = -\sigma_{ef}(N-1); \end{cases}$$

(The left part of the first equation in the set (6) is obtained as a geometric difference ΔV of microinclusion volume and the empty space volume in GaAs matrix). Here R_1 is GaAs matrix radius, P_L is Laplacian pressure, $\alpha(\varepsilon^{(1)})$ is QD (InAs) surface energy, which is the function of surface stress and QD deformation tensors [12]:

$$\alpha(\varepsilon^{(1)}) = \alpha(0) + \sum_{i,j} \sigma_{ij}^{(1)}\varepsilon_{ij}^{(1)} +$$

$$+ \frac{1}{2}\sum_{i,j,k,l} \varepsilon_{ij}^{(1)}(1) \cdot s_{ijkl}^{(1)} \cdot \varepsilon_{kl}^{(1)} + ...,$$

(7) where $\varepsilon_{ij}^{(1)}$, $\sigma_{ij}^{(1)}$ are respectively deformation tensor and surface stress tensor of QD; $s_{ijkl}^{(1)}$ is second-order stress tensor.

The solution of equation (5) is the following in case of spherical QD's:

$$u_r^{(1)} = C_1 r + \frac{C_2}{r^2}, \quad 0 \le r \le R_0, \qquad (8)$$

$$u_r^{(2)} = C_3 r + \frac{C_4}{r^2}, \quad R_0 \le r \le R_1. \qquad (9)$$

As in the dot $r = 0$ the displacement must be finite, then in the solution (8) let us assume $C_2 = 0$.

The field of displacements defines the following components of deformation tensor:

$$\varepsilon_{rr}^{(1)} = C_1, \qquad (10)$$

$$\varepsilon_{\varphi\varphi}^{(1)} = \varepsilon_{\theta\theta}^{(1)} = C_1, \qquad (11)$$

$$\varepsilon_{rr}^{(2)} = C_3 - \frac{2C_4}{r^3}, \qquad (12)$$

$$\varepsilon_{\varphi\varphi}^{(2)} = \varepsilon_{\theta\theta}^{(2)} = C_3 + \frac{C_4}{r^3}. \qquad (13)$$

We can find coefficients C_1, C_3, C_4 from the solution of the set (6), taking into account (1)–(4), (7)–(13).

The quasiparticle movement is considered in the superposition of Coulomb and deformation potential (Fig. 1). As one can see from Fig. 1, quantizing potential character is defined by the bottom of conduction band and QD heterostructure valence zone peak profiles. The energetic displacements of permitted bands edges influenced by elastic deformations are respectively the following [13]:

$$\Delta E_c^{(i)} = a_c^{(i)}\varepsilon^{(i)}(R_0, R_1);$$

$$\Delta E_\upsilon^{(i)} = a_\upsilon^{(i)}\varepsilon^{(i)}(R_0, R_1);$$

where $\varepsilon^{(i)}(R_0, R_1) = Sp\varepsilon^{(i)}$; $a_c^{(i)}$, $a_\upsilon^{(i)}$ are the constants of hydrostatic deformation potential of conduction band and valence band, respectively; $i = \begin{cases} 1 \equiv \text{InAs} \\ 2 \equiv \text{GaAs} \end{cases}$.

The potential energy of the electron and hole in the strained InAs QD in the
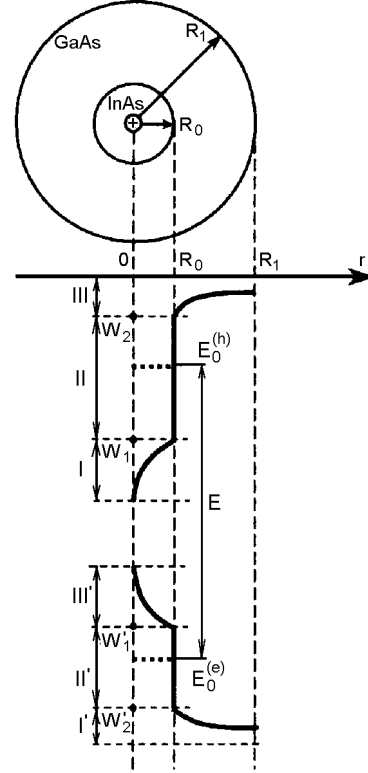

Fig. 1. The potential energy of electron and hole in coherent-strained InAs QD with ionized donor impurity. The potential energy is calculated from the top of the potential barrier of the quasiparticle in QD without impurities.

InAs/GaAs heterosystem is determined as follows:

$$U_{e,h}(r) = \begin{cases} -V^{(e,h)} - \dfrac{e^2}{4\pi\varepsilon_0\varepsilon_1 r}, & 0 \le r \le R_0, \\[2mm] -\dfrac{e^2}{4\pi\varepsilon_0\varepsilon_2 r}; & R_0 \le r \le R_1 \end{cases} \qquad (14)$$

where:

$$V^{(e)} = (\chi_1 - \chi_2) - a_c^{(1)} \cdot \varepsilon^{(1)}(R_0, R_1) + \quad (15)$$
$$+ a_c^{(2)} \cdot \varepsilon^{(2)}(R_0, R_1),$$

$$V^{(h)} = (\chi_2 + E_g^{(2)} - \chi_1 - E_g^{(1)}) + \quad (16)$$
$$+ a_\upsilon^{(1)} \cdot \varepsilon^{(1)}(R_0, R_1) - a_\upsilon^{(2)} \cdot \varepsilon^{(2)}(R_0, R_1).$$

Here χ_1, χ_2, $E_g^{(1)}$, $E_g^{(2)}$ are electron affinities and permitted band width of InAs and GaAs materials, respectively.

Energy transition into the fundamental state in a strained quantum dot is determined in the following way:

$$E(\varepsilon) = E_g^{(2)} - \left| a_c^{(2)} \cdot \varepsilon^{(2)}(R_0, R_1) \right| - \quad (17)$$

$$- \left| a_v^{(2)} \cdot \varepsilon^{(2)}(R_0, R_1) \right| - \left| E_0^{(e)} \right| - \left| E_0^{(h)} \right|,$$

where $E_0^{(e)}$, $E_0^{(h)}$ are the fundamental state energies of electron and hole in the strained QD, counted off the level of potential barrier peak, as shown in Fig. 1.

To determine charge carriers spectrum in the heterosystem under consideration, we need to solve Schrodinger equation

$$\left[-\frac{\hbar^2}{2}\nabla\frac{1}{m_{e,h}^*(\mathbf{r})}\nabla + U_{e,h}(r, R_0) \right]\Psi_{e,h}(\mathbf{r}) = \quad (18)$$

$$= E^{(e,h)}\Psi_{e,h}(\mathbf{r}).$$

The Schrodinger equation (18) in the spherical coordinates system is solved in the form:

$$\Psi_{nlm}(r,\Theta,\varphi) = R_{nl}(r) \cdot Y_{lm}(\Theta,\varphi). \quad (19)$$

Here $Y_{lm}(\Theta,\varphi)$ are spherical Legendre functions [14].

The analytic form of equation (18) solutions depends on the energy sections and heterosystem regions.

We shall find radial wave function $R(r)$ by changing to $\rho(r)$ function:

$$R(r) = \frac{\rho(r)}{r}. \quad (20)$$

Let us find the wave function of the electron in each of the energy sections I–III (Fig. 1) in different QD heterosystem regions.

1). Let us consider the case $0 \le r \le R_0$ (QD InAs medium).

The differential equation (18) for radial wave function with respect to (14), (15) will have the form:

$$\frac{d^2}{dr^2}R_1^{(e)}(r) + \frac{2}{r}\frac{dR_1^{(e)}(r)}{dr} - \frac{l(l+1)}{r^2}R_1^{(e)}(r) + \quad (21)$$

$$+ \frac{2m_{1_e}^*}{\hbar^2}\left(E^{(e)} + V^{(e)} + \frac{e^2}{4\pi\varepsilon_0\varepsilon_1 r} \right)R_1^{(e)} = 0.$$

Then we consider the solution of the equation (21) in cases $|E^{(e)}| > |V^{(e)}|$ and $|E^{(e)}| < |V^{(e)}|$.

a). $|E^{(e)}| > |V^{(e)}|$ (energy section I ($E^{(e)} < W_1$), $W_1 = -V^{(e)} - e^2/4\pi\varepsilon_0\varepsilon_1 R_0$ in Fig. 1).

After the following variables are introduced:

$$\xi_0 = \beta_0 r,$$

$$\beta_0 = i\left(\frac{8\,m_{1_e}^*(V^{(e)} + E^{(e)})}{\hbar^2} \right)^{\frac{1}{2}};$$

$$k_0 = i\frac{e^2}{4\pi\varepsilon_0\varepsilon_1\hbar}\left(\frac{m_{1_e}^*}{2(V^{(e)} + E^{(e)})} \right)^{\frac{1}{2}},$$

the equation (21) will be written as Whittaker equation:

$$\frac{d^2}{d\xi_0^2}\rho_1^{I^{(e)}}(r) + \quad (22)$$

$$+ \left(-\frac{1}{4} + \frac{k_0}{\xi_0} + \frac{1/4 - (l + 1/2)^2}{\xi_0^2} \right)\rho_1^{I^{(e)}}(r) = 0.$$

The solution of the equation (22) with respect to the finiteness of the wave function in the point $r = 0$ is expressed with hypergeometric function $_1F_1(a,b,x)$ [15]. Taking (20) into account, we obtain the following for the fundamental electron state

$$R_1^{I^{(e)}}(r) = \quad (23)$$

$$= C_1 \cdot \beta_0 \cdot \exp(-\beta_0 r/2) \cdot {_1F_1}(1 - k_0, 2, \beta_0 r).$$

b). $|E^{(e)}| < |V^{(e)}|$ (energy sections II ($W_1 < E^{(e)} < W_2$), energy sections III $W_2 < E^{(e)} < 0$), $W_2 = -e^2/4\pi\varepsilon_0\varepsilon_2 R_0$ in Fig. 1).

In this case, the equation (21) will take the form of Coulomb equation:

$$\frac{d^2}{d\xi_1^2}\rho_1^{II,III^{(e)}}(r) + \quad (24)$$

$$+ \left(1 - 2\frac{k_1}{\xi_1} + \frac{l(l+1)}{\xi_1^2} \right)\rho_1^{II,III^{(e)}}(r) = 0,$$

where

$$\xi_1 = \beta_1 r,$$

$$\beta_1 = \left(\frac{2m_{1_e}^*(V^{(e)} + E^{(e)})}{\hbar^2} \right)^{\frac{1}{2}};$$

$$k_1 = -\frac{e^2}{4\pi\varepsilon_0\varepsilon_1\hbar}\left(\frac{m_{1_e}^*}{2(V^{(e)} + E^{(e)})} \right)^{\frac{1}{2}}.$$

The solution of Coulomb equation (24) is Coulomb function [15]. Taking (20) into account, the solution for the fundamental electron state is as follows:

$$R_1^{II,III\,(e)}(r) = C_2 \cdot \frac{\exp(-\pi \cdot k_1/2) \cdot \Gamma(1 + ik_1)}{\Gamma(2)} \times$$

$$\times \beta_1 \cdot \exp(-i\beta_1 r) \cdot {}_1F_1(1 - ik_1, 2, 2i\beta_1 r). \quad (25)$$

2). Let us consider the case $R_0 \leq r \leq R_1$ (GaAs matrix).

Equation (18), with respect to (14), (16), will take the form:

$$\frac{d^2}{dr^2}R_2^{(e)}(r) + \frac{2}{r}\frac{dR_2^{(e)}(r)}{dr} - \frac{l(l + 1)}{r^2}R_2^{(e)}(r) + \quad (26)$$

$$+ \frac{2m_{2_e}^*}{\hbar^2}\left(E^{(e)} + \frac{e^2}{4\pi\varepsilon_0\varepsilon_2 r}\right)R_2^{(e)} = 0.$$

As in all the energy region (sections I–III in Fig. 1) $|E^{(e)}| > 0$, equation (26) can be written as Whittaker equation:

$$\frac{d^2}{d\xi_2^2}\rho_2^{I,II,III\,(e)}(r) + \quad (27)$$

$$+ \left(-\frac{1}{4} + \frac{k_2}{\xi_2} + \frac{1/4 - (l + 1/2)^2}{\xi_2^2}\right)\rho_2^{I,II,III\,(e)}(r) = 0.$$

where

$$\xi_2 = \beta_2 r,$$

$$\beta_2 = i\left(\frac{8m_{2_e}^* E^{(e)}}{\hbar^2}\right)^{\frac{1}{2}};$$

$$k_2 = i\frac{e^2}{4\pi\varepsilon_0\varepsilon_2\hbar}\left(\frac{m_{2_e}^*}{2E^{(e)}}\right)^{\frac{1}{2}}.$$

In this case, radial wave function for the electron in its fundamental state for energy sections I, II, III (Fig. 1) is a linear combination of hypergeometric functions ${}_1F_1(a_1, b_1, x)$ and $U(a_2, b_2, x)$ [15]:

$$R_2^{I,II,III\,(e)}(r) = \quad (28)$$

$$= C_3 \cdot \beta_2 \cdot \exp(-\beta_2 r/2) \cdot {}_1F_1(1 - k_2, 2, \beta_2 r) +$$

$$+ C_4 \cdot \beta_2 \cdot \exp(-\beta_2 r/2) \cdot U(1 - k_2, 2, \beta_2 r).$$

The conditions of wave functions continuity and probability flow density on QD-matrix boundary

$$\begin{cases} R_1^{(e,h)}(r)\big|_{r=R_0} = R_2^{(e,h)}(r)\big|_{r=R_0}, & (29) \\ \dfrac{1}{m_{1_{e,h}}^*}\dfrac{dR_1^{e,h}(r)}{dr}\bigg|_{r=R_0} = \dfrac{1}{m_{2_{e,h}}^*}\dfrac{dR_2^{(e,h)}(r)}{dr}\bigg|_{r=R_0}; \end{cases}$$

define $E^{(e,h)}$ spectre and wave functions of electron and hole in InAs/GaAs heterosystem with InAs quantum dots, together with

regularity condition of $R^{(e,h)}(r)$ function at $r \to 0$ and $r \to R_1$, and normalization consideration.

So, for energy section I: $E^{(e)} < W_1$, in which wave functions of the electron in InAs QD and GaAs matrix are determined respectively by the expressions (23) and (28), we obtain the following dispersion equation for calculating the energy of electron fundamental state:

$$a_{13}a_{21}a_{32} + a_{11}a_{22}a_{33} - \quad (30)$$

$$- a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} = 0.$$

In energy section II $W_1 < E^{(e)} < W_2$ (wave functions of the electron are determined by the expressions (25) and (28)) dispersion equation for the energy of electron fundamental state has the form:

$$a_{13}b_{21}a_{32} + b_{11}a_{22}a_{33} - \quad (31)$$

$$- b_{11}a_{23}a_{32} - a_{12}b_{21}a_{33} = 0,$$

where:

$$a_{11} = \beta_0 \cdot \exp(-\beta_0 R_0/2) \cdot {}_1F_1(1 - k_0, 2, \beta_0 R_0);$$

$$a_{12} = -\beta_2 \cdot \exp(-\beta_2 R_0/2) \cdot {}_1F_1(1 - k_2, 2, \beta_2 R_0);$$

$$a_{13} = -\beta_2 \cdot \exp(-\beta_2 R_0/2) \cdot U(1 - k_2, 2, \beta_2 R_0);$$

$$a_{21} = \frac{\beta_0^2 \cdot \exp(-\beta_0 R_0/2)}{2m_{1_e}^*} \times$$

$$\times \left((1 - k_0) \cdot {}_1F_1(2 - k_0, 3, \beta_0 R_0) - {}_1F_1(1 - k_0, 2, \beta_0 R_0)\right);$$

$$a_{22} = -\frac{\beta_2^2 \cdot \exp(-\beta_2 R_0/2)}{2m_{2_e}^*} \times$$

$$\times \left((1 - k_2) \cdot {}_1F_1(2 - k_2, 3, \beta_2 R_0) - {}_1F_1(1 - k_2, 2, \beta_2 R_0)\right);$$

$$a_{23} = -\frac{\beta_2^2 \cdot \exp(-\beta_2 R_0/2)}{2m_{2_e}^*} \times$$

$$\times \left((1 - k_2) \cdot U(2 - k_2, 3, \beta_2 R_0) - \frac{1}{2}U(1 - k_2, 2, \beta_2 R_0)\right);$$

$$a_{32} = \beta_2 \cdot \exp(-\beta_2 R_1/2) \cdot {}_1F_1(1 - k_2, 2, \beta_2 R_1);$$

$$a_{33} = \beta_2 \cdot \exp(-\beta_2 R_1/2) \cdot U(1 - k_2, 2, \beta_2 R_1);$$

$$b_{11} = \frac{\exp(-\pi \cdot k_1/2) \cdot \Gamma(1 + ik_1)}{\Gamma(2)} \times$$

$$\times \beta_1 \cdot \exp(-i\beta_1 R_0) \cdot {}_1F_1(1 - ik_1, 2, 2i\beta_1 R_0);$$

$$b_{21} = i\frac{\exp(-\pi \cdot k_1/2) \cdot \Gamma(1 + ik_1)}{\Gamma(2)} \times$$

$$\times \frac{\beta_1^2\exp(-i\beta_1 R_0)}{m_{1_e}^*}\left((1 - ik_1) \cdot {}_1F_1(2 - ik_1, 3, 2i\beta_1 R_0) - {}_1F_1(1 - ik_1, 2, 2i\beta_1 R_0)\right).$$

In energy section III $W_2 < E^{(e)} < 0$ the dispersion equation will be written in the
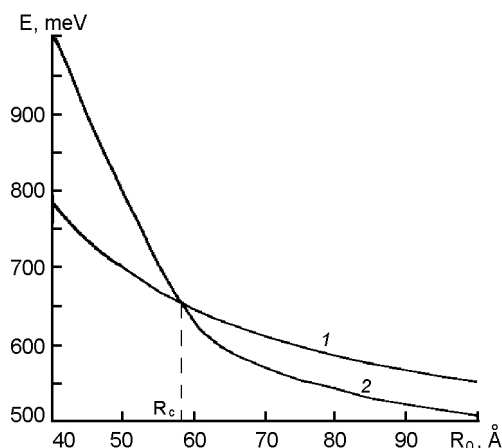
Fig. 2. The dependence of basic optical transition energy E in coherent-strained QD on its size R_0: *1* — the dependence $E(R_0)$ in QD without impurities; *2* — the dependence $E(R_0)$ in QD with ionized donor impurity.

form (32), as $R_1^{III^{(e)}}(r) = R_1^{II^{(e)}}(r)$, $R_2^{III^{(e)}}(r) = R_2^{II^{(e)}}(r)$.

Analogically we determine the spectre of $E^{(h)}$ and hole wave functions in InAs/GaAs heterosystem with InAs quantum dots, using continuity conditions (30) as well as function $R^{(h)}(r)$ regularity condition at $r \to 0$ and $r \to R_1$, and taking into account the normalization.

Fig. 2 shows numerical computation of E basic optical transition energy, in coherent-strained quantum dot InAs/GaAs (001) depending on its size R_0 with and without ionized Si donor impurity (curves 1 and 2, respectively, in Fig. 3). The calculation was made for InAs/GaAs nanoheterosystem with InAs QD at the following parameter values [16, 17]:

$a_1 = 6.08$ Å, $a_2 = 5.65$ Å,

$C_{11}^{(1)} = 0.833$ Mbar, $C_{11}^{(2)} = 1.223$ Mbar,

$C_{12}^{(1)} = 0.453$ Mbar, $C_{12}^{(2)} = 0.571$ Mbar,

$a_c^{(1)} = -5.08$ eV, $a_c^{(2)} = -7.17$ eV,

$a_\upsilon^{(1)} = 1$ eV, $a_\upsilon^{(2)} = 1.16$ eV,

$\chi_1 = 4.9$ eV, $\chi_2 = 4.07$ eV,

$E_g^{(1)} = 0.36$ eV, $E_g^{(2)} = 1.452$ eV,

$m_{1_e}^* = 0.057 m_0$, $m_{2_e}^* = 0.065 m_0$,

$m_{1_h}^* = 0.41 m_0$, $m_{2_h}^* = 0.45 m_0$,

$\alpha = 41$ meV/Å^2.

As one can see in Fig. 2, in case of quantum dot R_0 increase, the basic optical transition energy decreases monotonously, both with and without impurities, that is, optical transition shifts to long wavelength region.
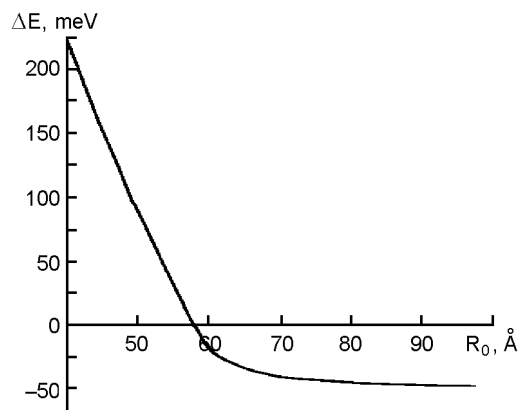

Fig. 3. The dependence of the basic optical transition energy shift on QD radius, caused by the presence of ionized donor impurity.

For smaller radiuses ($R_0 \sim 40$ Å $\div 57$ Å) the energetic width of E basic optical transition in quantum dots is larger with donor impurities than without them. In particular, at $R_0 = 40$ Å the main transition energy in coherent-strained QD without impurities is $E = 785.5$ meVB, while with an impurity it is 1005.2 meV. At large QD sizes $R_0 \geq 58$ Å the effect is the opposite.

The equality in $R_0 \geq 58$ Å corresponds to QD size, at which ionized donor centre of coherent-strained QD does not change the basic optical transition energy.

So the change of energetic width of the basic optical transition ($E = E^0 + \Delta E_\varphi + \Delta E_{def}$) in coherent-strained QD with ionized donor impurity with its size R_0 can be explained by different behaviour of the competing components ΔE_φ and ΔE_{def} with R_0 increase (E^0 is the component, corresponding to the basic optical transition energy in undeformed QD without donor impurities; ΔE_φ is the component of transition energy, induced by the presence of ionized donor impurity; ΔE_{def} is the component of transition energy, induced by impurity-free QD deformation potential).

The analysis of dependencies (14)–(16) shows that the potential energy of charge carriers in QD depends on its size in a non-monotonic way. Impurity implantation into QD leads to a substantial increase of potential well for electron as well as for hole in QD (for ~156 meV) compared to their values in QD without impurities (Fig. 1). At the same time, the potential well of both carriers reduces with the increase of radius QD R_0, and starting with $R_0 = 58$ Å increases

under the influence of deformation effects in smaller-sized QD's (40 $\overset{\circ}{A} \leq R_0 \leq 58$ $\overset{\circ}{A}$). So, in a quantum dot with ionized donor centre on QD sizes range 40 $\overset{\circ}{A} \leq R_0 \leq 58$ $\overset{\circ}{A}$ the electrostatic component of QD potential well deepens it for ΔU, which is smaller than the value of its reducing of depth caused only by deformation potential. The depth reducing of the well in QD size changing range $R_0 \sim 40$ $\overset{\circ}{A} \div 58$ $\overset{\circ}{A}$ leads to the increase of electron and hole energy levels in QD compared with their state in QD without impurities, which is accompanied by optical gap widening for QD with an impurity. Beyond this QD sizes range the opposite effect is observed: the wells deepening for both types of charge carriers. This is connected with the surface influence (Laplace pressure) decrease and complete deformation of QD lattice material. So, in large-sized QD's electron and hole levels decrease as to their levels without charged impurity. Fig. 3 shows the dependence of the basic optical transition energy shift on QD radius, defined by the presence of ionized donor impurity. The energy shift is calculated from the level of energy transition into the fundamental state in QD without impurities. Thus the region of negative energies corresponds to the range of QD radiuses ($R_0 \sim 58$ $\overset{\circ}{A} \div 100$ $\overset{\circ}{A}$), at which the optical gap of QD without the impurity is wider than with it. As we can see from Fig. 3, the energy transition shift into the fundamental state reduces monotonously with the increase of QD size. Here the shift value is more than in the case of smaller radius QD's (40 $\overset{\circ}{A} \leq R_0 \leq 58$ $\overset{\circ}{A}$). In particular, the value of the shift under consideration at QD radius $R_0 = 40$ $\overset{\circ}{A}$ is 219.6 meV, and if QD radius $R_0 = 100$ $\overset{\circ}{A}$, it is −44.1 meV.

Thus, the pre-calculated fundamental optical transition energy in coherent-strained QD with the ionized centre can be used, depending on its size, in the growing of quantum dots with electrically active centres. In particular, the problem solved lets us indicate the quantum dots sizes by photoluminescence spectres ($R_0 = R_c$, Fig. 2), at which the effect of these centres is compensated by deformation potential: as a result, these centres do not influence the basic optical transition energy.

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Вплив домішки на електронний перехід у когерентно-напруженій квантовій точці

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У рамках моделі деформаційного потенціалу досліджено вплив домішки на енергетичну ширину оптичної щілини квантової точки. Встановлено, що зі збільшенням розмірів квантової точки з іонізованою донорною домішкою оптична щілина звужується. Для менших радіусів ($R_0 \sim 40$ $\overset{\circ}{A} \div 57$ $\overset{\circ}{A}$) енергетична ширина основного оптичного переходу E у квантових точках з донорними домішками більша, ніж без домішок. У разі більших розмірів квантових точок $R_0 \geq 58$ $\overset{\circ}{A}$ спостерігається протилежний ефект.